Thermodynamics of a One-Dimensional System of Bosons with Repulsive Delta-Function Interaction

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(Received 10 October 1968)

The equilibrium thermodynamics of a one-dimensional system of bosons with repulsive delta-function interaction is shown to be derivable from the solution of a simple integral equation. The excitation spectrum at any temperature T is also found.

I. INTRODUCTION

The ground-state energy of a system of N bosons with repulsive delta-function interaction in one dimension with periodic boundary condition was calculated by Lieb and Liniger.[1] The Hamiltonian for the system is

$$H = -\sum_1^N \frac{\partial^2}{\partial x_i^2} + 2c\sum_{i>j}\delta(x_i - x_j), \quad c > 0, \quad (1)$$

and the periodic box has length L. Using Bethe's hypothesis[2] they showed that the k's in the hypothesis satisfy

$$(-1)^{N-1}\exp(-ikL) = \exp\left[i\sum_{k'}\theta(k' - k)\right], \quad (2)$$

where

$$\theta(k) = -2\tan^{-1}(k/c), \quad -\pi < \theta < \pi. \quad (3)$$

Taking the logarithm of (2) is a somewhat subtle process. In this paper we shall first discuss this point and show that *all* states of (1) are given by Bethe's hypothesis with real k's. The main purpose of the paper is to then evaluate the thermodynamical properties of the system at a finite temperature T.

While we try to maintain mathematical rigor in the rest of the paper, it is to be emphasized that Secs. III and IV are far from rigorous.

II. PROOF OF BETHE'S HYPOTHESIS FOR ALL STATES

We first take the logarithm of (2):

$$kL = 2\pi I_k + \sum_{k'}\theta(k - k'), \quad (4)$$

where

$$I_k = \text{integer}, \quad \text{if } N = \text{odd},$$
$$I_k + \tfrac{1}{2} = \text{integer}, \quad \text{if } N = \text{even}. \quad (5)$$

Now, for any set of real I's, $I_1, I_2, \cdots, I_N$, Eq. (4) has a unique real solution for the k's, $k_1, k_2, \cdots, k_N$. The proof of this statement (similar to but simpler than the proof of a corresponding statement[3] for the Heisenberg–Ising problem) follows. Let

$$\theta_1(k) = \int_0^k \theta(k)\,dk.$$

Define

$$B(k_1, \cdots, k_N) = \tfrac{1}{2}L\sum_1^N k_j^2 - 2\pi\sum_1^N I_j k_j - \tfrac{1}{2}\sum_{j,S}\theta_1(k_j - k_S). \quad (6)$$

Equation (4) is the condition for the extrema of B. Now the second-derivative matrix B_2 of B is positive-definite. [The first sum in (6) contributes a positive-definite part to B_2. The second sum contributes nothing. Each term in the third sum is negative-semidefinite, since $\theta_1''(k) = \theta'(k) < 0$.] Furthermore for large values of $\sum k^2$, $B \to \frac{1}{2}L(\sum k^2)$. Thus, B has *one* and *only one* extremum, namely, a minimum.

It is further clear from this argument that the solution above represents a point S in k space which moves continuously as c^{-1} is changed. [In fact, $dk_j/d(c^{-1})$ can be computed.] Now when $c^{-1} = 0$, $\theta_1 = 0$ and the minimum of B occurs at

$$k_j = 2\pi I_j/L. \quad (7)$$

Now the problem with $c^{-1} = 0$ is the problem of free particles with the condition that $\psi = 0$ whenever $x_i = x_j$ (any $i \neq j$). All eigenfunctions of H for this problem are easily seen to be the same as that of free fermions in the segment $0 \leq x_1 \leq x_2 \leq x_3 \leq \cdots \leq x_N \leq L$. Thus, when $c^{-1} = 0$, all eigenfunctions are of Bethe's form, with the k's given by (7) and with all the I's different.

* Partially supported by NSF Grant GP8731.
[1] E. Lieb and W. Liniger, Phys. Rev. **130**, 1605 (1963).
[2] H. A. Bethe, Z. Physik **71**, 205 (1931).
[3] C. N. Yang and C. P. Yang, Phys. Rev. **150**, 321 (1966).

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By a continuity argument with respect to c^{-1} we obtain the following:

Theorem: For any set of I's satisfying (5), no two of which are identical, there is a unique set of real k's satisfying (4), with no two k's being identical. With this set of k's, one eigenfunction of H, of Bethe's form, can be constructed. The totality of such eigenfunctions form a complete set for the boson system.

The numbers I are quantum numbers for the problem.

III. ENERGY AND ENTROPY FOR A SYSTEM WITH $N = \infty$

We now consider the problem for $N = \infty$ and $L = \infty$ at a fixed density $D = N/L$. For the ground state, the quantum numbers I/L form[1] a uniform lattice between $-D/2$ and $D/2$. The k's then form[1] a non-uniform distribution between a maximum k and a minimum k. For an excited state, (5) shows that the quantum numbers I/L are still on the same lattice, but not all lattice sites are taken, and the limits $-D/2$ and $D/2$ are no longer respected. We shall call the omitted lattice sites J_j/L. We would want to define corresponding "omitted k values" to be called holes. This can be easily done: Given the I's, Eq. (4) defines the set of k's as proved in the last section. Now,

$$Lh(p) \equiv pL - \sum_{k'} \theta(p - k') \tag{8}$$

is a continuous monotonic function of p. At $p = \pm\infty$, it is equal to $\pm\infty$. Those values of p where $Lh(p) = 2\pi I$ are k's. Those values of p where $Lh(p) = 2\pi J$ will be defined as holes.

For a large system, there is thus a density distribution of holes as well as one of k's:

$$\begin{aligned} L\rho(k)\,dk &= \text{No. of } k\text{'s in } dk, \\ L\rho_h(k)\,dk &= \text{No. of holes in } dk. \end{aligned} \tag{9}$$

By definition, the number of k's and holes in the interval dk is the number of times $Lh(k)$ ranges over values $2\pi I$ and $2\pi J$ in this interval.

Thus,

$$\frac{dh(k)}{dk} = 2\pi(\rho + \rho_h) \equiv 2\pi f(k). \tag{10a}$$

Equation (8) gives

$$h(k) = k - \int_{-\infty}^{\infty} \theta(k - k')\rho(k')\,dk'. \tag{10b}$$

Differentiation with respect to k gives

$$2\pi f = 2\pi(\rho + \rho_h) = 1 + 2c\int_{-\infty}^{\infty} \frac{\rho(k')\,dk}{c^2 + (k - k')^2}. \tag{11}$$

The energy per particle for the state is

$$E/N = D^{-1}\int_{-\infty}^{\infty} \rho(k)k^2\,dk, \tag{12}$$

where

$$D = N/L = \int_{-\infty}^{\infty} \rho(k)\,dk. \tag{13}$$

The entropy of the "state" is not zero since the existence of the omitted quantum numbers J_j allows many wavefunctions of approximately the same energy to be described by the same ρ and ρ_h. In fact, for given ρ and ρ_h, the total number of k's and holes in dk is $L(\rho + \rho_h)\,dk$, of which $L\rho\,dk$ are k's and $L\rho_h\,dk$ are holes. Thus the number of possible choices of states in dk consistent with given ρ and ρ_h is

$$\frac{[L(\rho + \rho_h)\,dk]!}{[L\rho\,dk]!\,[L\rho_h\,dk]!}.$$

The logarithm of this gives the contribution to the entropy from dk. Thus, the total entropy is, putting the Boltzman constant equal to 1,

$$\begin{aligned} S = \sum \{&(L\rho\,dk + L\rho_h\,dk)\ln(\rho + \rho_h) \\ &- L\rho\,dk \ln \rho - L\rho_h\,dk \ln \rho_h\} \end{aligned}$$

or

$$\begin{aligned} S/N = D^{-1}\int_{-\infty}^{\infty} &[(\rho + \rho_h)\ln(\rho + \rho_h) \\ &- \rho \ln \rho - \rho_h \ln \rho_h]\,dk. \end{aligned} \tag{14}$$

IV. THERMAL EQUILIBRIUM

At temperature T, we should maximize the contribution to the partition function from the states described by ρ and ρ_h. In other words, given ρ, ρ_h is defined by (11). One then computes the contribution to the partition function

$$\exp(S - ET^{-1}), \tag{14'}$$

where S and E are given by (14) and (12). The equilibrium ρ is then obtained by maximizing this contribution when ρ is varied subject to the condition (13).

The above described procedure leads in a straightforward manner to the following condition on the equilibrium ρ:

$$\begin{aligned} -A + k^2 + T\ln\frac{\rho}{\rho_h} \\ - \frac{Tc}{\pi}\int_{-\infty}^{\infty} \frac{dq}{c^2 + (k - q)^2} \ln\left(1 + \frac{\rho}{\rho_h}\right) = 0, \end{aligned}$$

where A is a Lagrange multiplier for the condition (13). Writing

$$\rho_h/\rho = \exp[\epsilon(k)/T], \tag{15}$$

we have

$$\epsilon(k) = -A + k^2 - \frac{Tc}{\pi}\int_{-\infty}^{\infty} \frac{dq}{c^2 + (k-q)^2} \times \ln\{1 + \exp[-\epsilon(q)/T]\}. \quad (16)$$

Equation (11) becomes

$$2\pi f(k) = 2\pi\rho(k)\{1 + \exp[\epsilon(k)/T]\} = 1 + 2c\int_{-\infty}^{\infty} \frac{\rho(q)\,dq}{c^2 + (k-q)^2}. \quad (17)$$

It will be shown in Appendix A that (16) can be solved for ϵ by iteration. Equation (17) is then a Fredholm equation for ρ. It will be shown in Appendix B that ρ can be obtained by iteration of (17). The energy, density D, and entropy can then be obtained from (12)–(14).

In Appendix C it will be shown that the maximization procedure that led to (16) can be more rigorously treated and that the conclusion of the next section can then be obtained without much algebra.

V. A = CHEMICAL POTENTIAL

We shall now show that A is the chemical potential. Multiply (16) with ρD^{-1} and integrate over k to obtain

$$A = D^{-1}\int_{-\infty}^{\infty} \rho(k^2 - \epsilon)\,dk + TD^{-1}\int_{-\infty}^{\infty} dq[(2\pi)^{-1} - f(q)] \times \ln\left(1 + \exp\left\{\frac{-\epsilon(q)}{T}\right\}\right). \quad (18)$$

In this formula, the square bracket is obtained from (17). Now use (15) to rewrite (14) as

$$S/N = D^{-1}\int_{-\infty}^{\infty} (\rho + \rho_h)\ln(1 + \exp\{-\epsilon/T\})\,dk + (DT)^{-1}\int_{-\infty}^{\infty} \rho\epsilon\,dk. \quad (19)$$

Thus, the free energy per particle is

$$FN^{-1} = (E - TS)N^{-1} = D^{-1}\int_{-\infty}^{\infty} (k^2 - \epsilon)\rho\,dk - TD^{-1}\int_{-\infty}^{\infty} (\rho + \rho_h)\ln[1 + \exp(-\epsilon/T)]\,dk. \quad (20)$$

Comparison of (18) and (20) gives, using $f = \rho + \rho_h$,

$$FN^{-1} = A - T(2\pi D)^{-1}\int_{-\infty}^{\infty} \ln[1 + \exp(-\epsilon/T)]\,dk. \quad (21)$$

If we now prove that the last term is $-PD^{-1}$ (where P is the pressure), then this formula demonstrates that A is the chemical potential, since by thermodynamics

$$F = -PL + N \times (\text{chemical potential}).$$

Now, by (21),

$$P = -\left(\frac{\partial F}{\partial L}\right)_T = -N\frac{\partial A}{\partial L} + \frac{TN}{2\pi D}\int_{-\infty}^{\infty} dq\,\frac{1}{1 + e^{\epsilon/T}}\left(-\frac{1}{T}\right)\frac{\partial\epsilon}{\partial A}\frac{\partial A}{\partial L} + \frac{T}{2\pi}\int_{-\infty}^{\infty} dk \ln(1 + e^{-\epsilon/T}), \quad (22)$$

where ϵ is considered a function of A defined by (16). Differentiating (16) with respect to A, we obtain

$$1 = -\left(\frac{\partial\epsilon}{\partial A}\right) + \frac{c}{\pi}\int_{-\infty}^{\infty} \frac{dq}{c^2 + (k-q)^2}\,\frac{(\partial\epsilon/\partial A)}{1 + e^{\epsilon(q)/T}}. \quad (23)$$

Comparing this equation with (17) we conclude, by the uniqueness of the solution of (17) (see Appendix B),

$$-\frac{\partial\epsilon}{\partial A} = 2\pi f(k) = 2\pi\rho(k)(1 + e^{\epsilon(k)/T}). \quad (24)$$

The first two terms in the expression (22) for P now cancel each other by (24) and (13). Thus,

$$P = \frac{T}{2\pi}\int_{-\infty}^{\infty} dk \ln(1 + e^{-\epsilon(k)/T}). \quad (25)$$

This proves the assertion that A is the chemical potential.

We shall prove in Appendix D that $P(A, T)$ is analytic in A and T. To recapitulate: ϵ is defined by (16) once A and T are given. Equation (25), then, gives P as a function of A and T. The other thermodynamical quantities are obtainable from the thermodynamical relation

$$dP = (S/L)\,dT + (N/L)\,dA. \quad (26)$$

If one wants to compute ρ, one uses either (17) or (24).

VI. SPECIAL CASES

A. $c = \infty$

The integrals in (16) and (17) do not contribute. Thus,

$$\epsilon = -A + k^2,$$
$$2\pi\rho = z\exp(-k^2/T)[1 + z\exp(-k^2/T)]^{-1},$$
$$2\pi\rho_h = [1 + z\exp(-k^2/T)]^{-1}, \quad (27)$$
$$P = T(2\pi)^{-1}\int_{-\infty}^{\infty} dk \ln[1 + z\exp(-k^2/T)],$$

where

$$z = \text{fugacity} = \exp(A/T).$$

These equations are those for a free Fermi gas, a result that is anticipated, as discussed in Sec. II.

B. $c = 0$

As $c \to 0$,

$$c(c^2 + x^2)^{-1} \to \pi\delta(x). \tag{28}$$

Thus, (16) gives

$$\epsilon = -A + k^2 - T \ln [1 + \exp(-\epsilon/T)]$$

or

$$\exp(-\epsilon/T) = [z^{-1} \exp(k^2/T) - 1]^{-1},$$

where we have used the fugacity defined in (27). Equation (25) now becomes

$$P = -T(2\pi)^{-1} \int_{-\infty}^{\infty} dk \ln [1 - z \exp(-k^2/T)]. \tag{29}$$

Equations (28) and (17) give

$$2\pi\rho_h = 1,$$
$$2\pi\rho = \exp(-\epsilon/T) = [z^{-1} \exp(k^2/T) - 1]^{-1}. \tag{30}$$

Equations (29) and (30) are precisely the corresponding expressions for a free Bose gas, as they should be.

C. $T = 0$

This is the case solved[1] by Lieb and Liniger.

It will be shown in Appendix A that $\epsilon(k)$ is a monotonically increasing function of k^2. At $T = 0$ assume the function to have a zero at $k^2 = q_0^2$ so that

$$\begin{aligned} &\epsilon(k) < 0, \quad k^2 < q_0^2, \\ &\epsilon(k) > 0, \quad k^2 > q_0^2, \\ &\epsilon(q_0) = 0. \end{aligned} \tag{31}$$

Equation (15) gives

$$\begin{aligned} &\rho = 0, \quad \text{for} \quad k^2 > q_0^2, \\ &\rho_h = 0, \quad \text{for} \quad k^2 < q_0^2. \end{aligned} \tag{32}$$

Equations (16) and (17) become

$$\epsilon(k) = -A + k^2 + \frac{c}{\pi} \int_{-q_0}^{q_0} \frac{\epsilon(q)\, dg}{c^2 + (k - q)^2}, \tag{33}$$

$$2\pi\rho = 1 + 2c \int_{-q_0}^{q_0} \frac{\rho(q)\, dq}{c^2 + (k - q)^2}, \quad \text{for} \quad k^2 < q_0^2. \tag{34}$$

Equation (34) is the equation[1] of Lieb and Liniger. Equation (33) will be useful in the next section.

VII. EXCITATION

Consider a state S, with I's and k's satisfying

$$k_j L = 2\pi I_j + \sum_i \theta(k_j - k_i), \tag{35}$$

and a state S', with primed I's and k's satisfying

$$k_j' L = 2\pi I_j' + \sum_i \theta(k_j' - k_i'). \tag{36}$$

We consider the case where

$$I_j' = I_j, \quad \text{except when} \quad j = \alpha. \tag{37}$$

[Notice that $I_1', I_2', \cdots, I_N'$ may *not* be a monotonically increasing series, since I_α' may be any integer for $N =$ odd and any integer $+\frac{1}{2}$ for $N =$ even.]

Subtract (35) from (36) to obtain

$$(k_j' - k_j)L = \sum_i [\theta(k_j' - k_i') - \theta(k_j - k_i)]. \tag{38}$$

We now assume that, for all $j \neq \alpha$, k_j and k_j' are approximately the same. This is the same assumption as used by Lieb[4] for the excitations near the ground state (i.e., $T = 0$). We write

$$(k_j' - k_j)L = \chi(k_j), \quad j \neq \alpha.$$

Thus, we expand those terms in (38) for which $i \neq \alpha$:

$$\chi(k_j) = \sum_{i \neq \alpha} \theta'(k_j - k_i)[\chi(k_j) - \chi(k_i)]L^{-1} + \theta(k_j - k_\alpha') - \theta(k_j - k_\alpha) \tag{39}$$

or

$$\chi(k) = \int_{-\infty}^{\infty} \theta'(k - q)[\chi(k) - \chi(q)]\rho(q)\, dq + \theta(k - k_\alpha') - \theta(k - k_\alpha). \tag{40}$$

Now we differentiate (10b) and use it to evaluate the coefficient of $\chi(k)$ in (40). Writing

$$f(k)\chi(k) = g(k), \tag{41}$$

we thus obtain

$$2\pi g(k) = -\int_{-\infty}^{\infty} \theta'(k - q)g(q) \times [1 + \exp\{+\epsilon(q)/T\}]^{-1}\, dq + \theta(k - k_\alpha') - \theta(k - k_\alpha) \tag{42}$$

or, explicitly,

$$g(k) = \frac{c}{\pi} \int_{-\infty}^{\infty} \frac{g(q)\, dq}{[c^2 + (k - q)^2][1 + \exp \epsilon(q)/T]} + \frac{1}{\pi} \tan^{-1}(k_\alpha' - k)c^{-1} - \frac{1}{\pi} \tan^{-1}(k_\alpha - k)c^{-1}. \tag{43}$$

This is a Fredholm integral equation which we shall write in operator form

$$g = \mathbf{K}g + G. \tag{44}$$

The momentum difference and energy difference

[4] E. Lieb, Phys. Rev. **130**, 1616 (1963).

between the two states are

$$\Delta K = \sum_j (k'_j - k_j) = k'_\alpha - k_\alpha + \int_{-\infty}^{\infty} \chi(k)\rho(k)\,dk \quad (45)$$

and

$$\Delta E = \sum_j (k'^2_j - k^2_j) = k'^2_\alpha - k^2_\alpha + \int_{-\infty}^{\infty} \chi(k)2k\rho(k)\,dk. \quad (46)$$

We shall prove in Appendix E the following:

Theorem: The momentum difference and energy difference[5] between the two states are

$$\Delta K = h(k'_\alpha) - h(k_\alpha) \quad (47)$$

and

$$\Delta E = \epsilon_0(k'_\alpha) - \epsilon_0(k_\alpha), \quad (48)$$

where

$$\epsilon_0 = \epsilon + A \quad (49)$$

and h is an odd function of k defined by (10a). These equations are accurate to the order N^0, not just N^1. (Notice that in evaluating the thermodynamical quantities, such as the energy, we only maintain accuracy up to the order N^1.)

VIII. DISCUSSIONS

(A) It is easy to prove that, for a finite number of simultaneous excitations,

$$\Delta K = \sum_\alpha h(k'_\alpha) - \sum_\alpha h(k_\alpha), \quad (50)$$

$$\Delta E = \sum_\alpha \epsilon_0(k'_\alpha) - \sum_\alpha \epsilon_0(k_\alpha). \quad (51)$$

Thus it is tempting to regard $h(k_\alpha)$ and $\epsilon_0(k_\alpha)$ as the momentum and energy of an elementary excitation.

To be more precise, we consider a system of noninteracting fermions with its single-particle states labeled by k. The momentum and energy of a single-particle state k are taken to be $h(k)$ and $\epsilon_0(k)$, respectively. The number of single-particle states in the k interval dk is $f(k)\,dk$. Such a system of particles will be called a model system M. At a fixed fugacity z, the model system has an average number of particles in the state k given by

$$ze^{-\epsilon_0/T}[1 + ze^{-\epsilon_0/T}]^{-1}, \quad (52)$$

so that the number of particles in the interval dk is $f\,dk$ times (52),which is also the same quantity in the true system. The model system M and the true system then have the same excitation spectra at T, *provided* only a finite number of excitations are made from thermal equilibrium. (Notice that the definition of the system M depends on h, ϵ_0, and f.)

(B) The excitation $k_\alpha \to k'_\alpha$ discussed in Sec. VII occurs with an excitation function which is proportional to a factor dependent on the method of excitation. But, in addition, it is also proportional to the number of I's in the interval dI near I_α and the number of vacancies in the interval dI' near I'_α. Thus, to excite

$$\text{from } (k \text{ in } dk) \text{ to } (k' \text{ in } dk')$$

there is an *intrinsic* excitation factor equal to

$$\rho(k)\rho_h(k')\,dk\,dk' = \rho(k)\rho(k')e^{\epsilon(k')/T}\,dk\,dk'. \quad (53)$$

APPENDIX A

We want to prove that (16) can be solved by iteration. Define the right-hand side of (16) as 0ϵ. Define further

$$\epsilon_1 = -A + k^2,$$
$$\epsilon_2 = 0\epsilon_1, \quad (A1)$$
$$\epsilon_3 = 0\epsilon_2, \quad \text{etc.}$$

It is easily seen that

$$\epsilon_1(k) > \epsilon_2(k) > \epsilon_3(k), \quad \text{etc.}$$

Next one can show that $\epsilon_n(k)$ is bounded from below. To do this, one proves first by induction that $\epsilon_n - k^2$ is a nondecreasing function of k^2. One then has

$$\epsilon_{n+1}(0) \geq -A - \frac{Tc}{\pi}\int_{-\infty}^{\infty} \frac{dq}{c^2 + q^2} \times \ln\,[1 + \exp\{-\epsilon_n(0)T^{-1} - q^2T^{-1}\}]. \quad (A2)$$

Now define the right-hand side of (A2) as $f[\epsilon_n(0)]$. That is,

$$f(x) = -A + x - \frac{Tc}{\pi}\int_{-\infty}^{\infty} \frac{dq}{c^2 + q^2} \ln\,(e^{x/T} + e^{-q^2/T}). \quad (A3)$$

It is clear from (A3) that $f(x) - x$ is monotonically decreasing. It has one and only one zero. Call the zero x_0 so that

$$f(x_0) = x_0. \quad (A4)$$

The right-hand side of (A2) shows that

$$f(x) \text{ is monotonically increasing} \quad (A5)$$

and that $f(x) < -A$. Thus (A4) gives

$$-A > f(x_0) = x_0. \quad (A6)$$

[5] In the limit $T \to 0$, the energy and momentum spectra are reducible to very simple expressions, using (31)–(34). These spectra have been obtained by Lieb in Ref. 4. Reduction to such simple equations as (33) is new.

Equations (A4), (A5), and (A6) show that

$$\epsilon_1(0) = -A > x_0,$$
$$\epsilon_2(0) \geq f[\epsilon_1(0)] > f(x_0) = x_0,$$
$$\epsilon_3(0) \geq f[\epsilon_2(0)] > f(x_0) = x_0, \quad \text{etc.}$$

Thus,

$$\epsilon_n(k) \geq \epsilon_n(0) > x_0. \tag{A7}$$

Having shown that

$$\lim_{n\to\infty} \epsilon_n(k) = \epsilon_L(k)$$

exists, one can next prove that the limit $\epsilon_L(k)$ does indeed satisfy (16). The main point is to show successively that (i), for $\epsilon > x_0$,

$$\frac{d}{d\epsilon} \ln (1 + e^{-\epsilon/T}) > -\frac{C}{T}, \quad \text{where} \quad 0 < C < 1,$$

and (ii) $\epsilon_n \to \epsilon_L$ uniformly in k.

APPENDIX B

To show that (17) can be solved by iteration we construct the symmetrized kernel

$$\mathbf{K}' = \frac{\pi^{-1}c}{c^2 + (k-q)^2} (1 + e^{\epsilon(q)/T})^{-\frac{1}{2}} (1 + e^{\epsilon(k)/T})^{-\frac{1}{2}}. \tag{B1}$$

If ψ is any normalized function and

$$\Phi = [1 + e^{\epsilon/T}]^{-\frac{1}{2}} \psi,$$

then

$$\psi^+ \mathbf{K}' \psi = \Phi^+ \frac{\pi^{-1}c}{e^2 + (k-q)^2} \Phi \leq \Phi^+ \Phi \leq [1 + e^{x_0/T}]^{-1} \psi^+ \psi,$$

where x_0 was defined in Appendix A. Thus, the eigenvalues of $\mathbf{K}'$ are less than unity and iteration of (17) converges.

The solution of (17) so obtained evidently satisfies

$$\rho > 0, \quad \rho_h = \rho \exp [\epsilon/T] > 0. \tag{B2}$$

APPENDIX C

(A) We treat the maximization procedure leading to (16) and (17) more rigorously here, showing that the solution of (16) and (17) indeed leads to a minimum of the free energy, i.e., a maximum of the partition function (14').

Consider any $\rho(k)$. If $\rho(k) \geq 0$ and the $\rho_h(k)$ defined by (11) is everywhere ≥ 0, we say that ρ is in R_0. It is clear that if ρ_1 and ρ_2 are both in R_0, then $x\rho_1 + (1-x)\rho_2$ for $0 \leq x \leq 1$ is also in R_0. Thus R_0 is convex.

We define $X(L, T, A, \rho)$ by

$$X = L\int_{-\infty}^{\infty} k^2 \rho \, dk + LT\int_{-\infty}^{\infty} [\rho \ln \rho + \rho_h \ln \rho_h - (\rho + \rho_h) \ln (\rho + \rho_h)] \, dk - LA\int_{-\infty}^{\infty} \rho \, dk. \tag{C1}$$

Consider $\rho = \rho_0 + x\rho_1$ where ρ_0 and ρ_1 are independent of x. Assume ρ to be in R_0 for a real segment of x. We can take the derivatives of X with respect to x in this segment. A straightforward calculation yields

$$\frac{dX}{dx} = L\int \rho_1 \, dk \Big[k^2 - A - \epsilon(k) - T \times \int B(k, q) \ln (1 + e^{-\epsilon(q)/T}) \, dq \Big], \tag{C2}$$

where ϵ is defined by

$$\exp (\epsilon/T) = \rho_h/\rho \tag{C3}$$

and

$$B(k, q) = \frac{\pi^{-1}c}{c^2 + (k-q)^2} = B(q, k). \tag{C4}$$

It is easy to show that

$$-T^{-1} \frac{\partial \epsilon(k)}{\partial x} = \rho^{-1}[1 + e^{-\epsilon/T}] \times \Big\{ \rho_1 - [1 + e^{\epsilon(k)/T}]^{-1} \int B(k, q) \rho_1(q) \, dq \Big\}. \tag{C5}$$

Now,

$$\frac{d^2X}{dx^2} = L\int \rho_1 \, dk \times \Big\{ -\frac{\partial \epsilon(k)}{\partial x} + \int B(k, q)(1 + e^{\epsilon(q)/T})^{-1} \frac{\partial \epsilon(q)}{\partial x} \, dq \Big\}. \tag{C6}$$

The double integral in (C6), after the switch $k \leftrightarrow q$, can be reduced through the use of (C5), giving

$$\frac{d^2X}{dx^2} = T^{-1}L\int \Big[\frac{\partial \epsilon(k)}{\partial x}\Big]^2 \rho(k)[1 + e^{-\epsilon(k)/T}]^{-1} \, dk > 0. \tag{C7}$$

By (B2), the solution of (16) and (17) gives a ρ in R_0. By (C2), at that ρ, $dX/dx = 0$.

We conclude further, from (C7), that X has a unique minimum in R_0 at the ρ given by (16) and (17).

(B) For given L, T, and A, we denote the minimum of X discussed above by $Y = Y(L, T, A)$. Clearly,

$$\frac{\partial Y}{\partial A} = -L\int \rho \, dk = -N,$$

$$\frac{\partial Y}{\partial T} = -S,$$

by (13) and (14). Further, since Y is proportional to L,

$$dY = -N\,dA - S\,dT + (Y/L)\,dL.$$

Thus,

$$d(Y + NA) = -S\,dT + (Y/L)\,dL + A\,dN.$$

But $Y + NA$ is the free energy. Thus,

$$A = \text{chemical potential}$$

and

$$Y/L = -\text{pressure}.$$

APPENDIX D

Write (16) symbolically in the form

$$\epsilon = W[A, T, \epsilon]. \tag{D1}$$

Consider two real numbers A_0, $T_0 > 0$ and let ϵ_1 be the solution of

$$\epsilon_1 = W[A_0, T_0, \epsilon_1]. \tag{D2}$$

The existence of ϵ_1 was proved in Appendix A. Now for complex values of A and T in the neighborhood of A_0, and T_0, we shall solve (D1) by iteration:

$$\epsilon_2 = W[A, T, \epsilon_1],$$
$$\epsilon_3 = W[A, T, \epsilon_2], \quad \text{etc.}$$

It can be shown that in a sufficiently small complex neighborhood R_1 of (A_0, T_0), $\epsilon_n \to \epsilon_\infty$ as $n \to \infty$, *uniformly* in k, T, and A. Since ϵ_n is analytic in A and T within R_1, so is ϵ_∞. It then easily follows that P as computed from (25) is analytic in A and T within R_1.

APPENDIX E

To prove (47) and (48) we define the kernel of (43):

$$K(k, q) = \frac{\pi^{-1}c}{[c^2 + (k - q)^2][1 + \exp \epsilon(q)/T]}. \tag{E1}$$

Equation (43) is then equivalent to

$$(\mathbf{1} - \mathbf{K})g = \int_{k_\alpha}^{k_{\alpha'}} K(k, q)[1 + \exp \epsilon(q)/T]\,dq. \tag{E2}$$

Let

$$(\mathbf{1} + \mathbf{L})(\mathbf{1} - \mathbf{K}) = \mathbf{1} \tag{E3}$$

or

$$\mathbf{L} - \mathbf{K} = \mathbf{LK}. \tag{E4}$$

Equation (E2) gives

$$g(k) = \int_{k_\alpha}^{k_{\alpha'}} L(k, q)[1 + \exp \epsilon(q)/T]\,dq. \tag{E5}$$

Now, the $\mathbf{K}'$ of (B1) is a symmetrical kernel with a symmetrical inverse kernel. From that fact we easily obtain

$$L(k, q)[1 + \exp \epsilon(q)/T] = L(q, k)[1 + \exp \epsilon(k)/T]. \tag{E6}$$

Two other useful formulas can be obtained as follows. Equation (17) can be rewritten as

$$(\mathbf{1} - \mathbf{K})f = (2\pi)^{-1}.$$

Operating with $1 + \mathbf{L}$ on both sides we obtain

$$f = (2\pi)^{-1} + (2\pi)^{-1}\int_{-\infty}^{\infty} L(k, q)\,dq. \tag{E7}$$

Similarly, differentiation of (16) with respect to k yields

$$\frac{d\epsilon}{dk} = 2k + \mathbf{K}\frac{d\epsilon}{dk}.$$

Thus,

$$\frac{d\epsilon}{dk} = 2k + \int_{-\infty}^{\infty} L(k, q)2q\,dq. \tag{E8}$$

Now, by (41),

$$\chi\rho = g/[1 + \exp(\epsilon/T)].$$

Thus, (45) becomes

$$\begin{aligned}\Delta K &= k_\alpha' - k_\alpha + \int_{-\infty}^{\infty} \frac{g(k)\,dk}{1 + \exp \epsilon(k)/T} \\ &= k_\alpha' - k_\alpha + \int_{-\infty}^{\infty} dk \int_{k_\alpha}^{k_{\alpha'}} dq L(k, q) \\ &\quad \times [1 + \exp \epsilon(q)/T][1 + \exp \epsilon(k)/T]^{-1} \\ &= k_\alpha' - k_\alpha + \int_{-\infty}^{\infty} dk \int_{k_\alpha}^{k_{\alpha'}} dq L(q, k) \\ &= k_\alpha' - k_\alpha + \int_{k_\alpha}^{k_{\alpha'}} dq[2\pi f(q) - 1],\end{aligned}$$

yielding (47). Similarly we derive (48).

APPENDIX F

We shall prove here rigorously that, for the ground state, the k's of Sec. II approach a distribution $L\rho(k)\,dk$ as $L \to \infty$, $N \to \infty$ proportionally. By continuing with respect to c^{-1} and the theorem of Sec. II, we know that for the ground state the I's form a close-packed set of integers or half-odd integers. We now define, as in (8),

$$h(k) = k - L^{-1}\sum_{k'} \theta(k - k'). \tag{F1}$$

Clearly,

$$\frac{dh}{dk} = 1 + \frac{2c}{L}\sum_{k'} \frac{1}{c^2 + (k - k')^2} > 1. \tag{F2}$$

Equation (F1) defines $h(k)$ for *all* real values of k. At the successive values of k_j, the successive values of $h(k_j)$ are $2\pi I_j/L$, by (4). Thus, the successive values of h form a lattice, with a lattice constant of $2\pi/L$, extending between $\pm(N - 1)\pi L^{-1}$. It is sometimes convenient to use h as the variable rather than k.

$k(h)$ is then a monotonically increasing odd function, defined for all real h, and approaches ∞ as $h \to \infty$.

Differentiation of (F1) gives, writing $dh/dk = h_1$,

$$h_1(k) = 1 + \frac{2c}{L}\sum_{k'}\frac{1}{c^2 + (k-k')^2}$$
$$= 1 + \frac{c}{\pi}\int_{-N\pi/L}^{N\pi/L}\frac{1}{c^2 + (k-k')^2}\,dh' + \text{residue}. \tag{F3}$$

The residue is in absolute value less than $A_1 L^{-1}$, since the integrand has a bounded derivative. Thus,

$$h_1(k) = 1 + \frac{c}{\pi} \times \int_{-Q}^{Q}\frac{1}{c^2 + (k-k')^2}\,h_1(k')\,dk' + O(L^{-1}), \tag{F4}$$

$$2N\pi/L = \int_{-Q}^{Q} h_1(k')\,dk'. \tag{F5}$$

It is now possible to complete the proof. We first use $h_1 > 1$ to obtain, from (F5),

$$Q < N\pi/L. \tag{F6}$$

With this fixed bound for Q, the inverse kernel for the integral equation (F4) is also absolutely bounded and we obtain

$$h_1(k) = 1(k, Q) + O(L^{-1}), \tag{F7}$$

where $1(k, Q)$ is the solution of (F4) when $O(L^{-1})$ is deleted. Integration of (F7) gives

$$2N\pi/L = \int_{-Q}^{Q} 1(k, Q)\,dk + O(L^{-1}). \tag{F8}$$

Thus, for fixed N/L, as $L \to \infty$, Q approaches a limit Q_0 given by

$$2\pi N/L = \int_{-Q_0}^{Q} 1(k, Q_0)\,dk. \tag{F9}$$

The rest is easy.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

On the Growth of the Number of Bound States with Increase in Potential Strength*

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(Received 21 November 1968)

For a wide class of potentials, it is shown that $N(\lambda)$, the number of bound states (including multiplicity) of $-\Delta + \lambda V$, obeys the conditions

$$A\lambda^{\frac{3}{2}} < N(\lambda) < B\lambda^{\frac{3}{2}}$$

for λ sufficiently large. A and B are positive finite numbers. In the centrally symmetric cases, a related growth condition on $l_{\max}(\lambda)$, the largest l channel with bound states, is also obtained, namely,

$$a\lambda^{\frac{1}{2}} < l_{\max}(\lambda) < b\lambda^{\frac{1}{2}}.$$

Finally, we discuss analogous results for a larger class of central potentials and for the many-body case.

I. INTRODUCTION

There are a fairly large number of results giving both lower and upper bounds on the number of bound states in a given l channel for a central potential.[1–8] From these, limits can be developed on the growth of the number of states in a fixed channel as the strength of the potential increases. The strongest general result of this nature has been obtained by Calogero.[4] If $n_l(\lambda V)$ is the number of bound states (not counting multiplicity) of angular momentum l for the operator $-\Delta + \lambda V$, then Calogero shows that

$$C\lambda^{\frac{1}{2}} < n_l(\lambda V) < D\lambda^{\frac{1}{2}}$$

for λ sufficiently large (λ will always be positive in this paper) and for a large class of potentials. C and D are, of course, V- and l-dependent (actually, D can be chosen independently of l).

For a restricted class of potentials (negative non-increasing as $r \to 0$), Chadan[6] has shown that

$$\lim_{\lambda \to \infty} n_l(\lambda V)/\lambda^{\frac{1}{2}}$$

exists and has a simple form in terms of V.

For some reason, there seem to be almost no results on the growth of the total number of bound states (counting multiplicity)

$$N(V) = \sum_{l=0}^{\infty} (2l + 1)n_l(V).$$

In this paper we show that, for a large class of not necessarily central potentials, there are nonzero constants A and B such that, for sufficiently large λ (Theorems 2, 3, and 6),

$$A\lambda^{\frac{3}{2}} < N(\lambda V) < B\lambda^{\frac{3}{2}}. \tag{1}$$

We also show (Theorems 1 and 5) that the number of angular-momentum channels with bound states goes as $\lambda^{\frac{1}{2}}$.

The conditions we impose on centrally symmetric V are the following:

(A) For all λ, $-\Delta + \lambda V$ has no eigenvalues of positive energy and the negative-energy spectrum is purely discrete of finite multiplicity.

(B) $I(V) \equiv \int_0^\infty dr \quad r\,|V(r)| < \infty$.

(C) $\inf [r^2 V(r)] \equiv -L > -\infty$.

(D) For some $\alpha > 0$, $\{r \mid V(r) < -\alpha\}$ has a non-empty interior.

The characterization of the negative spectrum in (A) can be assured by very weak conditions.[9] The absence of positive-energy bound states is assured by fairly mild conditions.[10]

(B) is the standard condition of Jost and Pais.[11] It can be replaced by the alternate condition:

(B′) V is minorized by a monotonically increasing potential $\tilde{V}$ with

$$Q(\tilde{V}) = \int_0^\infty dr\,|\tilde{V}(r)|^{\frac{1}{2}} < \infty.$$

* This research partially sponsored under Air Force Research and Development Command contract AF49(638)1545.

† National Science Foundation pre-doctoral fellow.

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We prove our results initially in the centrally symmetric case and discuss the easy extensions to the noncentral case in Sec. V.

II. THE UPPER BOUND

First we remark that there is an upper bound weaker than ours implicit in Bargmann's result[1] that

$$n_l(W) < I(W)/2l + 1 \tag{2}$$

for any potential W. For then $n_l(W) = 0$, if $2l + 1 > I(W)$, so that

$$N(W) < \sum_{l=0}^{[(I-1)/2]} (2l + 1)n_l(W) < I\{1 + [\tfrac{1}{2}(I - 1)]\} < \tfrac{1}{2}I(I + 1).$$

For $W = \lambda V$, $I(W) = \lambda I(V)$, so we see that

$$N(\lambda V) < \tfrac{1}{2}\lambda I(\lambda I + 1) < I^2\lambda^2, \quad \text{for} \quad \lambda > (I)^{-1}.$$

Our stronger result is obtained by a better estimate of the maximum l-channel with a bound state in it; we designate this l-value $l_{\max}(\lambda)$.

Theorem 1: If (A) and (C) hold, then for all λ,

$$l_{\max}(\lambda) < (L)^{\frac{1}{2}}\lambda^{\frac{1}{2}}.$$

Proof[12]*:* Since $-d^2/dr^2$ is a positive operator and $-\Delta + \lambda V$ has no positive eigenvalues, there are no bound states in the l channel, if

$$l(l + 1)/r^2 + \lambda V(r) > 0, \quad \text{for all } r.$$

But

$$l(l + 1)/r^2 + \lambda V > r^{-2}[l(l + 1) - \lambda L],$$

so $n_l(\lambda V) = 0$, if $l(l + 1) > \lambda L$; i.e., if $l > (\lambda L)^{\frac{1}{2}}$, then $n_l(\lambda V) = 0$, i.e., $l_{\max}(\lambda) < (\lambda L)^{\frac{1}{2}}$. Q.E.D.

Theorem 2: If (A), (B), and (C) hold, then, for all $\lambda > L^{-1}$,

$$N(\lambda V) < [2L^{\frac{1}{2}}I]\lambda^{\frac{3}{2}}.$$

Proof: By Bargmann's condition (2),

$$(2l + 1)n_l(\lambda V) < \lambda I,$$

so

$$N(\lambda V) < \sum_{l=0}^{l_{\max}} (2l + 1)n_l(\lambda V) < (\lambda I)(l_{\max} + 1) < (\lambda I)(\lambda^{\frac{1}{2}}L^{\frac{1}{2}} + 1) < 2\lambda^{\frac{3}{2}}IL^{\frac{1}{2}}$$

if $\lambda L > 1$. Q.E.D.

If (B′) holds instead of (B), we replace Bargmann's bound (2) with that of Calogero[2] (see also Ref. 7):

$$n_l(V) < (2/\pi)Q(\tilde{V}), \quad \text{for all } l. \tag{3}$$

Theorem 3: If (A), (B′), and (C) hold, then for all $\lambda > L^{-1}$,

$$N(\lambda V) < (8/\pi)LQ(\tilde{V})\lambda^{\frac{3}{2}}.$$

Proof: From Calogero's condition,

$$n_l(\lambda V) \leq \lambda^{\frac{1}{2}}[(2/\pi)Q(\tilde{V})],$$

so that

$$N(\lambda V) \leq \lambda^{\frac{1}{2}}\left[\frac{2}{\pi}Q(\tilde{V})\right] \sum_{l=0}^{l_{\max}} (2l + 1) = \lambda^{\frac{1}{2}}[(2/\pi)Q(\tilde{V})](l_{\max} + 1)^2 \leq \lambda^{\frac{3}{2}}[(8/\pi)LQ(\tilde{V})],$$

if $\lambda L \geq 1$.

III. A STRONG RAYLEIGH–RITZ PRINCIPLE

The nub of the proofs of the lower bounds is a form of the Rayleigh–Ritz principle which is more explicit than is usually found. While Theorem 4 is no doubt well known, its value for proving the existence of bound states does not seem to have been fully appreciated. It is essentially the principle used by Kato in his proof that the helium Hamiltonian has at least 25 585 bound states.[13]

Theorem 4: Let H be a self-adjoint operator on a domain D and let

$$\mu_n = \sup_{\Phi_1,\cdots,\Phi_{n-1}} \left\{ \inf_{\Psi \in U(\Phi_1,\cdots,\Phi_{n-1})} (\Psi, H\Psi) \right\},$$

where

$$U(\Phi_1, \cdots, \Phi_{n-1}) = \{\Psi \mid \Psi \in D, \|\Psi\| = 1 \text{ and } (\Phi_i, \Psi) = 0\}.$$

Then for each fixed n, either

(a) μ_n is the nth eigenvalue counting multiplicity or

(b) μ_n is the bottom of the essential spectrum and $\mu_n = \mu_{n+1} = \mu_{n+2} = \cdots$.

Moreover, there are at most $n - 1$ eigenvalues less than μ_n. (The essential spectrum is the set of points in the spectrum which are not isolated points of finite multiplicity.) The theorem holds if we replace D in the definition of U, by D_0, the domain of H as a bilinear form, i.e., the domain of $|H|^{\frac{1}{2}}$ as an operator.

We do not write out a proof of this theorem, as it is completely straightforward if one is willing to use a little spectral theory. The power of Theorem 4 comes when it is combined with condition (A); for if μ_n is negative and (A) holds, then (b) cannot be true and so (a) must hold. We remark that in application, H is either $-\Delta + V$ or $-\Delta + V$ restricted to an angular-momentum subspace.

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We first prove some corollaries which we need.

Corollary 1: If (D) holds, then $-\Delta + \lambda V$ has a bound p-state for λ sufficiently large.

Proof: Pick a smooth function ϕ of r of compact support, so that support of ϕ is contained in the set with $V(r) < 0$. Let $\Psi(r, \theta, \phi) = r\phi(r)Y_1^0(\theta, \phi)$. Then $(\Psi, V\Psi) < 0$ and so, for λ sufficiently large, $-(\Psi, \Delta\Psi) + \lambda(\Psi, V\Psi) < 0$, i.e., $-\Delta + \lambda V$ has a bound p-state.

Corollary 2: $n_l(\lambda V)$ is a monotonically increasing function of λ.

Proof:

$$-\Delta + \lambda_0 W = \lambda_0(-\Delta + W) + (1 - \lambda_0)(-\Delta).$$

For $\lambda_0 > 1$, $(1 - \lambda_0)(-\Delta)$ is a negative operator, so that by Theorem 4 applied to the operators on the space of functions of angular momentum l, $n_l(\lambda_0 W) \geq n_l(W)$, for all W. Letting $W = \lambda V$ and $\lambda_0\lambda = \lambda_1$, we see that $n_l(\lambda_1 V) \geq n_l(\lambda V)$ if $\lambda_1 > \lambda$.

Corollary 3: For any central potential V, and for $l \geq 1$,

$$n_l[\tfrac{1}{2}l(l+1)V] \geq n_1(V).$$

Proof:

$$-\frac{d}{dr^2} + \frac{l(l+1)}{r^2} + \frac{l(l+1)}{2}V = \frac{l(l+1)}{2}\left\{-\frac{d^2}{dr^2} + \frac{2}{r^2} + V\right\} + \frac{2 - l(l+1)}{2}\left(-\frac{d^2}{dr^2}\right), \quad (4)$$

where

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

is negative, so that the left-hand side of (4) has at least as many bound states as the right-hand side, i.e.,

$$n_l[\tfrac{1}{2}l(l+1)V] \geq n_1(V).$$

Corollary 4: Let V_1 obey condition (A) and let V_2 by any potential with $V_2(r) \geq V_1(r)$ for all r. If all the *negative-energy* eigenfunctions of $-\Delta + V_2$ are in the domain of $-\Delta + V_1$ as a bilinear form, then $N(\lambda V_1)$ is at least as large as the number of negative-energy eigenvalues of λV_2.

The proof is trivial; however, we remark that careful applications should not ignore the domain condition. We do not have a pathological V_2 in mind when we distinguish the negative-energy eigenvalues; rather we will not require V_2 to go to 0 at ∞ and, in fact, will take $V_2 \to \infty$ as $\mathbf{r} \to \infty$.

IV. THE LOWER BOUNDS

Theorem 5: Let V obey (A) and (D) and suppose $n_1(\lambda_0 V) \geq 1$. Then, for $\lambda > \lambda_0$,

$$l_{\max}(\lambda) \geq (\tfrac{1}{2}\lambda_0^{-\frac{1}{2}})\lambda^{\frac{1}{2}}.$$

[*Note:* By Corollary 1, (D) implies that some λ_0 exists.]

Proof: By Corollary 3,

$$n_l[\tfrac{1}{2}\lambda_0 l(l+1)V] \geq 1.$$

Thus, if $\lambda \geq \frac{1}{2}\lambda_0 l(l+1)$, $n_l(\lambda V) \geq 1$ (by Corollary 2). Thus, if $l \leq (\lambda/\lambda_0)^{\frac{1}{2}}$ and $l \geq 1$, $n_l(\lambda V) \geq 1$; i.e.,

$$l_{\max}(\lambda) \geq \left[\left(\frac{\lambda}{\lambda_0}\right)^{\frac{1}{2}}\right] \geq \frac{1}{2}\left(\frac{\lambda}{\lambda_0}\right)^{\frac{1}{2}}, \quad \text{if} \quad \lambda \geq \lambda_0.$$

Corollary 5: If V obeys conditions (A) and (D), then, for all $\lambda \geq \lambda_0$ (λ_0 as in Theorem 5),

$$N(\lambda V) > \lambda/\lambda_0.$$

Proof:

$$N(\lambda) > \sum_{l=0}^{l_{\max}}(2l+1) = (l_{\max}+1)^2 \geq \{[(\lambda/\lambda_0)^{\frac{1}{2}}] + 1\}^2 \geq \lambda/\lambda_0. \qquad \text{Q.E.D.}$$

To get an improvement on the growth rate of Corollary 5, a comparison with specific potentials seems necessary. A comparison proof is also possible for obtaining the upper bounds.

Lemma 1: Let D be the region of $\mathbb{R}^3$ with

$$|x - x_0| < L, \quad |y - y_0| < L, \quad |Z - Z_0| < L,$$

and let

$$V_0(r) = \begin{cases} -P, & x \in D, \\ \infty, & x \in D, \end{cases} \quad \text{with} \quad P > 0.$$

Let $N(\lambda V_0)$ be the number of bound states of negative energy for $-\Delta + \lambda V_0$. Then for λ sufficiently large,

$$N(\lambda V_0) > A\lambda^{\frac{3}{2}}.$$

Proof: The eigenvalues of $-\Delta + \lambda V_0$ are

$$E_n(\lambda) = (\pi/2L)^2(n_1^2 + n_2^2 + n_3^2) - \lambda P,$$

where n_1, n_2, n_3 are positive integers. Thus, $N(\lambda V_0)$ asymptotically approaches the volume of an octant of a sphere of radius $C\lambda^{\frac{1}{2}}$. As a result, $N(\lambda V_0)/\lambda^{\frac{3}{2}}$ actually approaches a limit which is positive.

Theorem 6: Let V obey (C) and (D) and suppose $D(H_0 + \lambda V) \supset D(H_0) \cap D(V)$, where $D(X)$ is the domain of X *as a bilinear form.* Then, for λ sufficiently large:

$$N(\lambda V) \geq A\lambda^{\frac{3}{2}}.$$

Proof: Pick a ball B in $\mathbb{R}^3$ so that $V(\mathbf{r}) < -P$ in B. Inside B, find a region D as in Lemma 1 and let V_0 be as in that lemma. The eigenfunctions for the square well are in $D(V)$ by (C) and they are in $D(H_0)$ [they are *not* in the domain of H_0 as an operator; to be in $D(H_0)$, they need only possess L^2 first derivatives]; thus, from the domain condition, Corollary 4, and Lemma 1, the theorem follows. Q.E.D.

We remark first that condition (C) is much stronger than what we need. It is sufficient that V be negative in some ball B for which

$$\int_B |V(\mathbf{r})|^2 \, d^3r < \infty.$$

We also remark that it is almost inconceivable that one can make sense out of $H_0 + V$ without having the domain condition hold. Examples of classes of V for which it must hold are:

(1) $V \in L^2 + L^\infty$ (Kato potentials);

(2) V bounded below, $H_0 + \lambda V$ defined by the Friedrichs' extension method;

(3) $V \in L^\infty + L^{\frac{3}{2}}$, in which case one can show that $H_0 + \lambda V$ is bounded below and so Friedrichs' extension can be used.

V. EXTENSIONS TO MORE GENERAL CASES

To N dimensions: It is a little enlightening to note that in N dimensions $\lambda^{\frac{3}{2}}$ is replaced by $\lambda^{N/2}$; for example, our comparison potential, the harmonic oscillator, has $N(\lambda V_0) \sim \lambda^{N/2}$. Thus, we can understand the fact $n_l(\lambda V) \sim \lambda^{\frac{1}{2}}$ by realizing that the single-channel Schrödinger equation is essentially 1-dimensional.

To noncentral potentials: The proof of Theorem 6 carries over without change to the noncentral case. To obtain an upper bound, we need only a simple comparison potential. Let

$$V_{\min}(r) = \min_{|\mathbf{r}|=r} V(\mathbf{r}).$$

Then, since $V_{\min} < V$, we have $N(\lambda V_{\min}) > N(\lambda V)$. If $V_{\min}$ obeys (A), (B), and (C), the upper bound given by Theorem 2 yields an upper bound for $N(\lambda V)$.

To the many-body case: As with most problems in nonrelativistic potential theory, things really get interesting in the many-body case. Also as with most problems, the two-body methods are not capable of extension. In this case, there are negative-energy continua (due to relative motion of bound clusters) which complicate the analysis and invalidate all the arguments we have used in the two-body case.

ACKNOWLEDGMENTS

It is a pleasure to thank Professor V. Bargmann and Professor A. S. Wightman for their interest and perceptive comments.

Super Hilbert Space and the Quantum-Mechanical Time Operators

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(Received 26 September 1967)

The basic idea of super Hilbert space is to represent physical states by continuous linear functionals on a space of good functions, rather than by functions in a Hilbert space. Since L_2 is in one-to-one correspondence with a subset of super Hilbert space, everything that can be done in L_2 can be done in super Hilbert space. In addition, however, it is possible to have a time operator and thus to base relativistic quantum mechanics on covariant four-dimensional commutation relations.

1. INTRODUCTION

There has always been a certain tension in modern physics caused by the fact that special relativity demands that space and time be treated on an equivalent footing, whereas nonrelativistic quantum mechanics (and ultimately all quantum mechanics) is based upon the three-dimensional commutation relation

$$[\hat{p}, \hat{q}] = -i\hbar. \tag{1.1}$$

The fourth component of the commutation relation in (1.1) would naturally be

$$[\hat{H}, \hat{T}] = -i\hbar, \tag{1.2}$$

where $\hat{H}$ is the Hamiltonian and $\hat{T}$ is a Hermitian time operator.

As Pauli[1] pointed out long ago, no such operator can exist in Hilbert space. The reason for this is the following: If $\hat{T}$ is a Hermitian operator in Hilbert space and α is a real number, then $\exp(i\alpha\hat{T})$ is a unitary operator in Hilbert space. (In fact, every continuous one-parameter group of unitary transformations $\{\mu_\alpha\}$ in Hilbert space can be written $\mu_\alpha = \exp(i\alpha\hat{A})$, for some Hermitian operator $\hat{A}$.[2]) Then, if $\hat{T}$ satisfies (1.2) for some Hermitian operator $\hat{H}$ and ψ_E is an eigenfunction of $\hat{H}$ with eigenvalue E, $\exp(i\alpha\hat{T})\psi_E$ is an eigenfunction of $\hat{H}$ with eigenvalue $E + \alpha\hbar$. Since α is an arbitrary real number, then, if $\hat{T}$ is a Hermitian operator in Hilbert space and satisfies (1.2), $\hat{H}$ must have a continuum of eigenvalues from $-\infty$ to $+\infty$. The result of this old argument is that for any Hermitian operator in Hilbert space $\hat{H}$ which does not have a continuum of eigenvalues from $-\infty$ to ∞, no Hermitian operator $\hat{T}$ exists in Hilbert space which satisfies (1.2).

We call pairs of operators which satisfy (1.2) canonical conjugates. It is not only the Hamiltonian which has no canonical conjugate, but also such operators as the z component of the angular momentum and the number operator. In fact, $\hat{q}$ and $\hat{p}$ and linear combinations of them are the only operators which do have canonical conjugates in Hilbert space.

In the "super Hilbert space" which is developed in Sec. 2, the above argument does not hold and we show in Sec. 3 how to construct a canonical conjugate for a broad class of operators. In Secs. 4 and 5 we discuss the classical and quantum-mechanical time operators and solve for them explicitly for the free particle and the harmonic oscillator. In Sec. 6, we discuss the time-delay operator in scattering theory. In Sec. 7 some comments are made on relativistic quantum mechanics in super Hilbert space. In Secs. 8 and 9 we discuss norms and the uncertainty principle, respectively.

The basic idea of the super-Hilbert-space treatment of quantum mechanics is to consider the state of a quantum-mechanical system to be represented by a continuous linear functional on a space M, rather than by a function. Since there is an isomorphism between L_2 and a subset of all the continuous linear functionals on the M's chosen, everything that can be done in L_2 can be done in super Hilbert space, but the reverse is not true.

Commonly used functions, such as $\exp(ikx)$, $|x|$, and $\delta(x)$, do not exist in L_2. Furthermore, even though Hamiltonians containing potentials which are inverse powers of x are commonly considered operators, inverse powers of the operators $\hat{p}$ and $\hat{q}$ are not operators in L_2. For example, if we define $\hat{q}$ by $\hat{q}^\beta f(x) \equiv x^\beta f(x)$ for all β and $f(x)$, then for any $\beta > 0$ we can find an α such that $x^{-\alpha}\exp(-x^2) \in L_2$, but $\hat{q}^{-\beta}x^{-\alpha}\exp(-x^2) = x^{-\alpha-\beta}\exp(-x^2) \notin L_2$. We have only to pick α so that $\frac{1}{2} > \alpha > \frac{1}{2} - \beta$. The argument is the same in three dimensions except that $\frac{1}{2}$ is replaced by $\frac{3}{2}$. In super Hilbert space, the existence of all the derivatives of every member is guaranteed and all the commonly used functions, such as $\exp(ikx)$, $|x|$, and $\delta(x)$, can be represented as functionals in super Hilbert space.

[1] W. Pauli, *Handbuch der Physik*, Vol. 24/1, p. 143.
[2] F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Frederick Ungar Publ. Co., New York, 1955), p. 385.

The real importance, however, of the super-Hilbert-space formulation of quantum mechanics lies in the ability to base the difference between classical and quantum mechanics on four-dimensional commutation relations, such as $[\hat{p}^\mu, \hat{q}_\nu] = -i\hbar\delta^\mu_\nu$. From this basis it may be possible to construct a natural and manifestly covariant relativistic quantum mechanics.

2. THE MATHEMATICAL STRUCTURE

In the interests of simplicity and clarity we discuss the structure based on L_2 and consider only one-dimensional space. The results can easily be extended to any Hilbert space.

Consider first the set S of functions which are everywhere differentiable any number of times and such that they and all their derivatives fall off at infinity faster than the inverse of any polynomial. We call such functions "good functions," after Lighthill.[3] Under the usual concept of convergence in L_2, S is an everywhere-dense subset of L_2. In this paper, however, we define convergence in any linear function space M which contains S as follows. $\{\Phi_n\}$, a sequence of functions in M, is said to converge to a function $\Phi(x)$, if—for all j (including zero), in every bounded region in which $\Phi(x)$ has j derivatives—the first j derivatives of all the Φ_n exist and converge uniformly to the corresponding derivatives of $\Phi(x)$, and if the Φ_n satisfy the condition that the constants C_{km} $(m \leq j;\ k = 0, 1, 2, \cdots)$ in

$$\left| x^k \frac{d^m}{dx^m} \Phi_n(x) \right| \leq C_{km} \tag{2.1}$$

can be chosen independent of n in every closed set in which $\Phi(x)$ is defined and has m derivatives. $\pm\infty$ are counted as points in the definition of "closed" here.

Consider the space M^* of functions which are the complex conjugates of the functions in M. If M and M^* contain the same elements, we call M "symmetrical." We assume that all function spaces used in this paper are symmetrical. A linear symmetrical space of functions which includes S will be called a "fine" space.

The dual space of M, M', is the set of all continuous linear functionals on M. In order to make this meaningful, we must define "continuous." The dependence of a general element of $M^\dagger$, called a "generalized function," on the space M can be written $F(f)$ or (F, f), where f is an element of M and F is the particular functional in $M^\dagger$. For a particular f and F, (F, f) is a complex number. A linear functional F is said to be continuous at f if the

$$\lim_{n\to\infty} (F, f_n) = (F, f) \tag{2.2}$$

for every sequence of functions in M, $\{f_n\}$, which converges to f. It is a well-known theorem of functional analysis[4] that if a linear functional F is continuous at some point (f_0) of M, then it is continuous everywhere in M.

A given generalized function F is defined on some space $M \supseteq S$, which we call the "domain" of F and write as $\mathfrak{D}(F)$. A sequence of generalized functions $\{F_n\}$ is said to converge to the generalized function F if $\mathfrak{D}(F_n) \supseteq \mathfrak{D}(F)$ for all F_n and if, for every $f(x)$ in $\mathfrak{D}(F)$,

$$\lim_{n\to\infty} (F_n, f) = (F, f). \tag{2.3}$$

Let $\mathfrak{W}$ be the set of all continuous linear functionals whose domain is a fine space. Addition of two elements in $\mathfrak{W}$ is defined by

$$(F_1 + F_2, f) \equiv (F_1, f) + (F_2, f), \tag{2.4}$$

for arbitrary f in $\mathfrak{D}(F_1) \cap \mathfrak{D}(F_2)$. Multiplication of an element of $\mathfrak{W}$ by a complex number α is defined by

$$(\alpha F, f) \equiv \alpha^* (F, f), \tag{2.5}$$

for arbitrary f in $\mathfrak{D}(F)$, where the * denotes complex conjugation. Multiplication of an element in $\mathfrak{W}$ by a complex infinitely differentiable function $a(x)$, bounded by some polynomial, is defined by

$$(a(x)F, f) \equiv (F, a^*(x)f), \tag{2.6}$$

for arbitrary f such that $a^*(x)f \in \mathfrak{D}(F)$. F^* is defined by

$$(F^*, f) \equiv (F, f^*)^*, \tag{2.7}$$

for arbitrary f such that $f^* \in \mathfrak{D}(F)$.

We now define the bilinear form (f, F) where the element on the left comes from M and the element on the right from $M^\dagger$ by

$$(f, F) \equiv (F, f)^*. \tag{2.8}$$

Note that (F, f) as defined above is a symmetric bilinear form. As such it fulfills all the requirements of an inner product except that, since the left and right components are drawn from different spaces, the additional requirement of being strictly positive has no meaning here. We now proceed to give it a meaning.

We can define a "natural" one-to-one correspondence between the elements of the space S and a subset of elements in $\mathfrak{W}$. This can be seen as follows. With every function $f(x)$ in S we can associate a functional

[3] M. J. Lighthill, *Fourier Analysis and Generalized Functions* (Cambridge University Press, Cambridge, England, 1959).

[4] A. N. Kolmogorov and S. V. Fomin, *Elements of the Theory of Functions and Functional Analysis* (Graylock Press, Rochester, 1957), Vol. I, p. 77.

F in $\mathfrak{W}$ whose domain is S, by

$$(F, \Phi) = \int_{-\infty}^{\infty} f^*(x)\Phi(x)\,dx, \tag{2.9}$$

for every function Φ in S, where the integral is a Riemann integral. The integral in (2.9) converges for every $f(x)$ and $\Phi(x)$ in S. Let W be the set of all complex-valued functions defined on a subset of the real line. We will define the zero elements in W and $\mathfrak{W}$ by

$$(F, 0) = 0; \quad (0, f) = 0, \tag{2.10}$$

for all F in $\mathfrak{W}$ and f in W. Through (2.9) a given f in S has a unique counterpart F in $\mathfrak{W}$. If there were in S two functions, f_1 and f_2, which both had the same counterpart in $\mathfrak{W}$, then from (2.9),

$$\int_{-\infty}^{\infty} (f_2^*(x) - f_1^*(x))\Phi(x)\,dx = 0 \tag{2.11}$$

for every $\Phi(x)$ in S. But one such $\Phi(x)$ is $f_2(x) - f_1(x)$. Thus,

$$\int_{-\infty}^{\infty} |f_2(x) - f_1(x)|^2\,dx = 0. \tag{2.12}$$

Since $f_2(x) - f_1(x)$ satisfies (2.12), is continuous everywhere, and goes to zero faster than the inverse of any polynomial, then $f_2(x) = f_1(x)$ everywhere. Thus we have proved that there is a one-to-one correspondence between the elements of S and the elements of a subset of $\mathfrak{W}$ defined by (2.9). If F_1 is an element of $\mathfrak{W}$ and is in one-to-one correspondence with an element f_1 of S through (2.9), we say that F_1 and f_1 are "counterparts" of one another. In the same way we could show that there is a one-to-one correspondence between a subset $\mathfrak{L}_2$ of $\mathfrak{W}$ and L_2. In fact, the substitution of $f(x)$ for $f^*(x)$ on the right-hand side of (2.9) defines an isomorphism between $\mathfrak{L}_2$ and L_2.

The analog of the strictly positive requirement in the definition of an inner product can now be given. If F_1 is an element of $\mathfrak{W}$ which has a counterpart f_1 in S, then we define (F_1, Φ) by

$$(F_1, \Phi) \equiv \int_{-\infty}^{\infty} f_1^*(x)\Phi(x)\,dx, \tag{2.13}$$

for all Φ in S. It then follows that

$$(F_1, f_1) \geq 0 \tag{2.14}$$

for all f_1 in S and $(F_1, f_1) > 0$, unless $f_1(x) \equiv 0$. Thus (F, f) is a generalized inner product. For the purposes of this paper we refer to it as the inner product. In order to clarify which element is in which space we henceforth write (F, f) as $\langle F | f)$, the angular bracket indicating that the element inside is in $\mathfrak{W}$ and the round bracket indicating that the element inside is in $\mathfrak{D}(F)$. To simplify the notation further we adopt a Dirac-type notation and write elements in W as $|f)$ and elements in $\mathfrak{W}$ as $\langle F|$. Using this notation we write the counterpart of $|f)$ in $\mathfrak{W}$ as $\langle f|$.

There is a one-to-one correspondence between M and M^*. If $f(x) \in M$, then we put $f^*(x)$ in M^* in correspondence with it. We write the vector in M^* which corresponds to $|f(x))$ in M as $(f(x)|$. The space of all continuous linear functionals on M^* we denote by $(M^*)^\dagger$. Since there is a one-to-one correspondence between M and M^*, there is a one-to-one correspondence between $M^\dagger$ and $(M^*)^\dagger$. We write the vector in $(M^*)^\dagger$ which corresponds to $\langle g|$ in $M^\dagger$ as $|g\rangle$. The particular correspondence is that which makes [see (2.8)]:

$$\langle g\,|f(x)) = (f(x)\,|\,g\rangle^*, \tag{2.15}$$

for every $|f(x))$ in $\mathfrak{D}(\langle g|)$. Thus $|f(x))$, $(f(x)|$, $|f\rangle$, and $\langle f|$ are in one-to-one correspondence and are called "counterparts" of one another.

Note that neither $|f(x))$ nor $|f\rangle$ is a Dirac ket vector. $|f(x))$ is a function of x in W and $|f\rangle$ is a linear functional in $\mathfrak{W}^*$, whereas the Dirac ket $|\psi\rangle$ is a linear functional on a Hilbert space. [We nonetheless call $|f\rangle$ a ket and $\langle f|$ a bra. Perhaps we should call $(f|$ an arb and $|f)$ a tek.] Thus for any $|g(x))$, $|h(x))$, $|g(x))\,|h(x)) = |g(x)h(x))$. $|g\rangle\,|f\rangle$, however, has no meaning.

Since there is an isomorphism between L_2 and a subset of $\mathfrak{W}$, we call $\mathfrak{W} \oplus \mathfrak{W}^*$ "super Hilbert space" and denote it by $\mathfrak{Z}$. We denote the space $W \oplus W^*$ by Z.

The derivative $\langle dh/dx|$ of a generalized function $\langle h|$ is defined by

$$\left\langle \frac{dh}{dx} \middle| \Phi(x) \right) \equiv -\left\langle h \middle| \frac{d\Phi}{dx} \right), \tag{2.16}$$

for every $|\Phi(x))$ such that $d\Phi/dx \in \mathfrak{D}(\langle h|)$.

We define an operator as a linear mapping from a subspace of $\mathfrak{Z}$ into $\mathfrak{Z}$. Since the domain of an operator may be smaller than its range, we must take care in applying an operator more than once.

The operators $\hat{q}$ and $\hat{p}$ are defined as follows:

$$\hat{q}\,|f\rangle \equiv |xf\rangle; \quad \hat{p}\,|f\rangle \equiv i\hbar(d/dx)\,|f\rangle. \tag{2.17}$$

We now show that (2.17) is sufficient to define $\hat{q}$ on all of $\mathfrak{W}^*$. If $|f\rangle$ is any ket in $\mathfrak{W}^*$, it is easy to show that $|xf\rangle$ is linear on $\mathfrak{D}(|xf\rangle)$. Further, since for any $(g|$ in S^*, $(xg|$ is in S^* and, since $(g\,|\,xf\rangle = (xg\,|f\rangle$, it follows that $|xf\rangle$ is defined on every $(g|$ in S^*. It remains to be shown that $|xf\rangle$ is continuous on S^*.

If $g^{(k)}$ is the kth derivative of g,

$$|(xg_n)^{(k)} - (xg)^{(k)}| = \left| \sum_{j=0}^{1} \binom{k}{j} x^{(j)}(g_n^{(k-j)} - g^{(k-j)}) \right| \leq \sum_{j=0}^{1} \binom{k}{j} |x^{(j)}|\,|g_n^{(k-j)} - g^{(k-j)}|. \quad (2.18)$$

Thus if $\{g_n^{(k)}\}$ converges uniformly to $g^{(k)}$ for all k in every bounded interval, $\{(xg_n)^{(k)}\}$ converges uniformly to $(xg)^{(k)}$ for all k in every bounded interval. Also, since

$$|x^k(xg_n)^{(m)}| = |x^k(xg_n^{(m)} + mg_n^{(m-1)})| \leq |x^{k+1}g_n^{(m)}| + m\,|x^k g_n^{(m-1)}|, \quad (2.19)$$

if $\{g_n\}$ satisfies (2.1), $\{xg_n\}$ also satisfies (2.1). Thus if $\{g_n\}$ converges to g, $\{xg_n\}$ converges to xg. It follows that the continuity of $|xf\rangle$ on S is assured by the continuity of $|f\rangle$. Therefore, for all $|f\rangle$ in $\mathfrak{W}^*$, $|xf\rangle$ is in $\mathfrak{W}^*$ and the domain of $\hat{q}$ is indeed all of $\mathfrak{W}^*$. The corresponding proof that (2.17) defines $\hat{p}$ on all of $\mathfrak{W}^*$ is even easier and will be left to the reader.

We denote by $\mathcal{S}$ the set of elements in $\mathfrak{W}$ which are in one-to-one correspondence with S through (2.9). Since the domain of $\hat{q}$ and $\hat{p}$ is all of $\mathfrak{W}^*$, any polynomial in $\hat{p}$ and $\hat{q}$ is an operator. It is also true that any polynomial in $\hat{p}$ and $\hat{q}$ takes an element in $\mathcal{S}^*$ into an element in $\mathcal{S}^*$. But $d|f\rangle/dx = i\hat{A}\,|f\rangle$ does not in general imply $|f\rangle = \exp(ix\hat{A})\,|f\rangle$, for some $|f(0)\rangle$, even if $\hat{A}$ is independent of x, since $\exp(ix\hat{A})$ is an infinite expansion.

We denote the complement of $\mathcal{S}$ in $\mathfrak{W}$ by $\mathfrak{W} - \mathcal{S}$. We now show that there exist operators generated by $\hat{x}$ and $\hat{p}$ which take any element in $\mathcal{S}^*$ into $\mathfrak{W}^* - \mathcal{S}^*$. Consider the operator defined on $\mathcal{S}^*$ by

$$\hat{D}^{(N)} = N^{\frac{1}{2}} \exp(-N\hat{q}^2). \quad (2.20)$$

For any $|f\rangle$ in $\mathcal{S}^*$

$$\hat{D}^{(N)}\,|f\rangle = |N^{\frac{1}{2}} \exp(-Nx^2)f\rangle. \quad (2.21)$$

$|N^{\frac{1}{2}} \exp(-Nx^2)f\rangle$ is in $\mathcal{S}^*$ for any $N > 0$. We show, however, that the $\lim_{N\to\infty} \hat{D}^{(N)}\,|f\rangle$ is in $\mathfrak{W}^* - \mathcal{S}^*$.

For any $(g(x)|$ in $\mathcal{S}^*$,

$$\begin{aligned} &|(g(x)|\,(N/\pi)^{\frac{1}{2}} \exp(-Nx^2)f\rangle - f^*(0)g(0)| \\ &= \left| \int_{-\infty}^{\infty} \left(\frac{N}{\pi}\right)^{\frac{1}{2}} \exp(-Nx^2) f^*(x)g(x)\,dx - f^*(0)g(0) \right| \\ &= \left| \int_{-\infty}^{\infty} \left(\frac{N}{\pi}\right)^{\frac{1}{2}} \exp(-Nx^2)(f^*(x)g(x) - f^*(0)g(0))\,dx \right| \\ &\leq \max \left| \frac{d}{dx}(f^*(x)g(x)) \right| \int_{-\infty}^{\infty} \left(\frac{N}{\pi}\right)^{\frac{1}{2}} \exp(-Nx^2)\,|x|\,dx \\ &= \max \left| \frac{d}{dx}(f^*(x)g(x)) \right| (\pi N)^{-\frac{1}{2}} \to 0, \quad \text{as} \quad N \to \infty. \end{aligned} \quad (2.22)$$

Thus $\hat{D}^{(\infty)}$ exists as an operator and

$$\pi^{-\frac{1}{2}} \hat{D}^{(\infty)}\,|f\rangle = |f(x)\delta\rangle, \quad (2.23)$$

where $|f(x)\delta\rangle$ has the property that, for any $|g(x))$ in S,

$$\langle f(x)\delta\,|\,g(x)) = \langle \delta\,|\,f^*(x)g(x)) = f^*(0)g(0). \quad (2.24)$$

We define the linear functional $\langle\delta|$ on all $f(x)$ defined at $x = 0$ by

$$\langle \delta\,|\,f(x)) \equiv f(0). \quad (2.25)$$

Thus there exist operators generated by $\hat{q}$ and $\hat{p}$ which take elements of $\mathcal{S}^*$ into elements of $\mathfrak{W}^* - \mathcal{S}^*$.

In addition, there exist denumerable combinations of $\hat{q}$ and $\hat{p}$ which are not operators at all. For example,

$$\hat{E}^{(N)} \equiv \sum_{j=0}^{N} \frac{1}{j!}\,\hat{q}^{2j} \quad (2.26)$$

is a well-defined operator for any N. It takes any $|f\rangle$ in $\mathcal{S}^*$ into

$$\left| \sum_{j=0}^{N} \frac{1}{j!}\,\hat{q}^{2j} f \right\rangle$$

in $\mathcal{S}^*$ which is defined for any $(g(x)|$ in S^* by

$$\left(g(x) \left| \sum_{j=0}^{N} \frac{1}{j!}\,\hat{q}^{2j} f \right\rangle = \sum_{j=0}^{N} \frac{1}{j!} \int_{-\infty}^{\infty} dx x^{2j} f(x) g^*(x). \quad (2.27)$$

The operator

$$\hat{E}^{(\infty)} \equiv \lim_{N\to\infty} \hat{E}^{(N)} = \sum_{j=0}^{\infty} \frac{1}{j!}\,\hat{q}^{2j} \quad (2.28)$$

does not exist, however, since $\hat{E}^{(\infty)}\,|\exp(-\alpha x^2)\rangle = |\exp[(1-\alpha)x^2]\rangle$, which is not in general in $\mathfrak{W}^*$, since $(\exp(-\beta x^2)|$ is in S^*, but

$$(e^{-\beta x^2} \,|\, e^{(1-\alpha)x^2}\rangle = \int_{-\infty}^{\infty} dx e^{(1-\alpha-\beta)x^2} \quad (2.29)$$

does not converge for $(\alpha + \beta) \leq 1$.

A. Inverse Functionals

In order to understand inverse operators we must first understand inverse functionals and the process of the regularization of functions with removable singularities.

By removable singularity we mean that, if $f(x)$ has a singularity at $x = y$ and if $|x - y| < \epsilon$, then $|f(x)| < |x - y|^{-N}$ for some $N(\epsilon)$.

Let $f(x)$ be a function locally summable everywhere except at x_0, where it has a nonsummable singularity [for example, $f(x) = x^{-1}$]. Then in general,

$$F(\Phi) = \int_{-\infty}^{\infty} f^*(x)\Phi(x)\,dx, \quad \Phi(x) \in S$$

will diverge. The integral will converge, however, if $\Phi(x)$ vanishes in a neighborhood of $x = x_0$. A functional with the same value as F for every $\Phi(x)$ in its domain which vanishes in a neighborhood of x_0 is called a regularization of f. Gel'fand and Shilov[5] show that every function $f(x)$ which has at most a finite number of removable singularities can be regularized. It is also true that no function having an infinite number of singularities in any finite interval can be regularized.

We now define a "quasigood" function as any function $f(x)$ which has the following properties:

(1) $f(x)$ is regularizable.
(2) Every derivative of $f(x)$ is regularizable.
(3) There exist real numbers ϵ and $N(\epsilon)$ such that if $|x| > \epsilon$, then $|f(x)| < |x|^N$.

It follows that if $f(x)$ is a quasigood function, every derivative of $f(x)$ is a quasigood function.

E is said to be a "regularization rule" for a set of regularizable functions C, if for every function $f(x)$ in C, E defines a unique generalized function $\langle \mathcal{R}(E,f)|$ on a fine space (which is the same for all functions in C), such that

$$\langle \mathcal{R}(E,f) \mid \Phi) = \int_{-\infty}^{\infty} f^*(x)\Phi(x)\,dx \qquad (2.30)$$

for every $\Phi(x)$ in its domain which vanishes in a neighborhood of every locally nonsummable singularity of $f^*(x)$. $\langle \mathcal{R}(E,f)|$ is here called the regularization of $f(x)$ according to rule E.

We now show that there is a one-to-one correspondence between a subset $\mathfrak{F}_i$ of $\mathfrak{W}$ and a set of equivalence classes of functions J_i, which are regularizable by rule E_i. Let J_i include only functions which have at most a finite number of discontinuities in any finite interval. Since $\langle \mathcal{R}(E_i,f)|$, $f \in J_i$, is by definition a unique functional, it remains to be shown only that for two distinct (i.e., from different equivalence classes) functions in C, $f_1(x)$ and $f_2(x)$, $\langle \mathcal{R}(E_i,f_1)| \neq \langle \mathcal{R}(E_i,f_2)|$. Let $\Phi(x)$ be a function in $\mathfrak{D}(\langle \mathcal{R}_i,f|)$ which vanishes in a neighborhood of every locally nonsummable singularity of $f_1^*(x)$ and $f_2^*(x)$. Then if $\langle \mathcal{R}(E_i,f_1)| = \langle \mathcal{R}(E_i,f_2)|$ on $\mathfrak{D}(\langle \mathcal{R}(E_i,f)|)$, we have

$$\int_{-\infty}^{\infty} (f_1^*(x) - f_2^*(x))\Phi(x)\,dx = 0 \qquad (2.31)$$

for every such $\Phi(x)$.

The function $f_1(x) - f_2(x)$ has a finite number of singular points in any finite region. Let z be a nonsingular point of $f_1(x) - f_2(x)$. Then $f_1(x) - f_2(x)$ is continuous in some neighborhood of z. Assume $f_1(z) - f_2(z) \neq 0$. Then in some neighborhood, $z - \epsilon < x < z + \epsilon$, $f_1(x) - f_2(x)$ is continuous and everywhere positive or everywhere negative. But if we pick

$$\sigma(z) = \frac{f_1(z) - f_2(z)}{|f_1(z) - f_2(z)|};$$

$$\Phi(x) \equiv \sigma(z) \exp\left[-\frac{\epsilon^2}{\epsilon^2 - (x-z)^2}\right], \qquad (2.32)$$

$$\text{for} \quad z - \epsilon \leq x \leq z + \epsilon,$$

$$\equiv 0, \quad \text{elsewhere},$$

the integral in (2.31) is greater than zero. Thus $f_1(z) - f_2(z) = 0$ and $f_1(z) = f_2(z)$ except at most of the finite number of points at which $[f_1(z) - f_2(z)]$ is not defined. The equivalence classes are thus made of those functions which differ only on a set of measure zero. Q.E.D.

Let J be the set of all quasigood functions. We can divide J into mutually exclusive sets J_i, such that J_i in J is in one-to-one correspondence with $\mathfrak{F}_i$ in $\mathfrak{W}$. The $\mathfrak{F}_i$ are not necessarily disjoint. We denote by $\mathfrak{F}$ the union of all these $\mathfrak{F}_i$. We denote $J \cup J^*$ by K. And defining $\mathfrak{F}^*$ to have the same relation to J^* as $\mathfrak{F}$ has to J, we denote $\mathfrak{F} \cup \mathfrak{F}^*$ by $\mathfrak{K}$.

Let Q_{n-1} be the set of all functions which are everywhere differentiable any number of times and which rise less fast than x^{n-1} as $|x| \to \infty$. There are many regularizations of x^{-n}. The most obvious is given by defining $\langle x^{-n}|$ on Q_{n-1} by

$$\langle x^{-n} \mid \Phi) \equiv \int_{-\infty}^{\infty} dx x^{-n}\left\{\Phi(x) - \sum_{m=0}^{n-1} (x^m/m!)\Phi_{(0)}^{(m)}\right\}, \qquad (2.33)$$

where $\Phi_{(0)}^{(m)} \equiv [(d^m/dx^m)\Phi(x)]_{(x=0)}$.

It is easy to show that $\langle x^{-n}|$ is linear on Q_{n-1}. In view of the linearity of Q_{n-1}, it is then sufficient to show that $\langle x^{-n}|$ is continuous at $x = 0$. Let $\{\Phi_t\}$ be a sequence in Q_{n-1} which converges to zero.

If we let

$$A_t(x) \equiv \Phi_t(x) - \sum_{m=0}^{n-1} (x^m/m!)\Phi_{t(0)}^{(m)} \equiv B_t + iC_t, \qquad (2.34)$$

where $B_t \equiv \text{Re}\,(A_t)$ and $C_t \equiv \text{Im}\,(A_t)$, then B_t and C_t can be written in the form[5]

$$B_t(x) = \Phi_{tr}^{(n)}(x_1)x^n/n!; \quad C_t = \Phi_{ti}^{(n)}(x_1)x^n/n!, \qquad (2.35)$$

where Φ_{tr} is the real part of Φ_t, Φ_{ti} is the imaginary part of Φ_t, and $0 < x_1 < x$.

[5] I. M. Gel'fand and G. E. Shilov, *Generalized Functions, Vol. 1* (Academic Press Inc., New York, 1964), Chap. I.

For any $b > 0$,

$$\langle x^{-n} \mid \Phi_t) = \int_{-\infty}^{-b} dx x^{-n} A_t(x) + \int_b^{\infty} dx x^{-n} A_t(x) + \int_{-b}^{b} dx x^{-n} A_t(x). \quad (2.36)$$

Since $\int_{-\infty}^{\infty} dx x^{-n} A_t(x)$ converges, for any given t we can make b sufficiently large so that the absolute value of the sum of the first two integrals on the right-hand side of (2.36) is less than $\epsilon/2$. Also,

$$\int_{-b}^{b} dx x^{-n} A_t(x) = \frac{1}{n!} \int_{-b}^{b} dx \Phi_{tr}^{(n)}(x_1(x)) + \frac{i}{n!} \int_{-b}^{b} dx \Phi_{ti}^{(n)}(x_1(x)). \quad (2.37)$$

Since $\{\Phi_t\}$ converges to zero, for any given b we can find t sufficiently large so that

$$|\Phi_t^{(n)}(x_1)| < n! \, \epsilon/(8b). \quad (2.38)$$

It follows that

$$|\Phi_{tr}^{(n)}(x_1)| < n! \, \epsilon/(8b); \quad |\Phi_{ti}^{n}(x_1)| < n! \, \epsilon/(8b). \quad (2.39)$$

Thus, for any given b, we can make t sufficiently large so that

$$\int_{-b}^{b} dx x^{-n} A_t(x) < \frac{\epsilon}{2}.$$

Thus if $\{\Phi_t\}$ converges to zero, it follows that for any given ϵ we can find a t sufficiently large so that

$$\langle x^{-n} \mid \Phi_t) < \epsilon. \quad (2.40)$$

Thus, $\langle x^{-n}|$ is continuous on Q_{n-1}.

B. Adjoint Operators, Compatible Spaces, and Eigenvalues

We have previously shown that any polynomial in $\hat{x}$ and $\hat{p}$ maps from $\mathcal{S}$ into $\mathcal{S}$. Similarly, any finite combination of positive or negative integer powers of $\hat{x}$ and $\hat{p}$ map from $\mathcal{K}$ into $\mathcal{K}$.

Let G be any set in $\mathfrak{Z}$. G^* will denote the set whose elements are the counterparts in $\mathfrak{Z}$ of those in G. It follows that for any such G, $G^{**} = G$. Though the * operation here is really counterpart conjugation, it is analogous to complex conjugation in Z, and we call it complex conjugation here also. With this usage it follows that $(M^\dagger)^* = (M^*)^\dagger$, and we here drop the parentheses and write just $M^{\dagger *}$ or $M^{*\dagger}$.

If $\hat{A}\,|f\rangle \in M^{*\dagger}$, then $(\hat{A}\,|f\rangle)^* \in M^\dagger$. We define $\hat{A}^*$ by

$$\langle f|\,\hat{A}^* \equiv (\hat{A}\,|f\rangle)^*. \quad (2.41)$$

Since $(\hat{A}\,|f\rangle)^{**} = (\langle f|\,\hat{A}^*)^* = \hat{A}\,|f\rangle$, it is natural to define $\hat{A}^{**} \equiv \hat{A}$. Also it follows from (2.8) that for any $|f\rangle$ and $(g|$,

$$\langle f|\,\hat{A}^*\,|g) = (g|\,\hat{A}\,|f\rangle^*. \quad (2.42)$$

If X is a set of functions, and Y is a set of continuous linear functionals each of whose domain includes X, then X is said to be "in the domain of" Y.

Let F and G be fine sets of functions. Let $\mathcal{F}$ and $\mathcal{G}$ be sets of continuous linear functionals such that F is in the domain of $\mathcal{G}$ and G is in the domain of $\mathcal{F}$. Let $\langle g| \in \mathcal{G}$; $|g) \in G$; $\langle f| \in \mathcal{F}$; $|f) \in F$. If it is possible to establish a one-to-one correspondence between $\mathcal{F}$ and F, where $|f)$ denotes the function corresponding to $\langle f|$, and a one-to-one correspondence between $\mathcal{G}$ and G, where $|g)$ denotes the function corresponding to $\langle g|$, such that

$$\langle g\,|f) = \langle f\,|\,g)^* \quad (2.43)$$

for all $|f)$ in F and $|g)$ in G, then F, G, $\mathcal{F}$, and $\mathcal{G}$ are said to be "compatible." Note that $|f)$ is not necessarily in the domain of $\langle f|$. If $F = G$ and $\mathcal{F} = \mathcal{G}$, F and $\mathcal{F}$ are said to be "self-compatible." For example, L_2 is self-compatible. An example of compatible but not self-compatible spaces is provided by the following. If J_i is a set of functions including S which are regularizable by rule E, and $\mathfrak{J}_i$ is a subset of $\mathfrak{W}$, which is in one-to-one correspondence with J_i through putting $\langle f| \equiv \langle \mathcal{R}(E,f)|$ as in (2.30), then if $F = J_i$; $\mathcal{F} = \mathfrak{J}_i$; $G = S$; and if $\mathcal{G}$ is defined as the set of all $\langle g|$ defined by (2.43), then J_i, $\mathfrak{J}_i$, S, and $\mathcal{G}$ are compatible.

Using (2.15), which defined $|f\rangle$ in terms of $\langle f|$, (2.43) can be written

$$\langle g\,|f) = (g\,|f\rangle. \quad (2.44)$$

Let F, G, $\mathcal{F}$, and $\mathcal{G}$ be compatible sets. $\hat{A}$ is said to be "Hermitian" or "self-adjoint" on these compatible sets if

$$(g|\,\hat{A}\,|f\rangle = \langle g|\,\hat{A}^*\,|f), \quad (2.45)$$

for all $\langle f|$ in $\mathcal{F}$ and $\langle g|$ in $\mathcal{G}$.

$|f\rangle$ will be called the solution to

$$\hat{A}\,|f\rangle = |g\rangle, \quad (2.46)$$

if and only if

$$(h|\,\hat{A}\,|f\rangle = (h\,|\,g\rangle \quad (2.47)$$

for all $(h|$ in $\mathfrak{D}(|g\rangle)$. The eigenvalue equation for $\hat{A}$ is

$$\hat{A}\,|f\rangle = \beta\,|f\rangle, \quad (2.48)$$

where the number β is an eigenvalue and $|f\rangle$ is an eigenket. Equation (2.48) implies

$$\langle f|\,\hat{A}^* = \langle f|\,\beta^*. \quad (2.49)$$

If $\langle f|$ is a member of some set of functionals that is self-compatible, then (2.48) and (2.49) together imply

$$(f|\,\hat{A}\,|f\rangle - \langle f|\,\hat{A}^*\,|f) \equiv (\beta - \beta^*)(f\mid f\rangle. \quad (2.50)$$

It follows that if $\hat{A}$ is self-adjoint on a self-compatible set of functionals, the eigenvalues of $\hat{A}$ associated with eigenkets in the set are real.

C. The Fourier Transformation

Two functionals that play very special roles are the Fourier transformation and the $\langle\delta|$. The Fourier transform of every $|f(x))$ in S is in S. In fact,[6] the Fourier transformation maps S onto S. If every element of a space D has a Fourier transform, we call D a "Fourier space." We call the space whose elements are the Fourier transforms of D the "Fourier transformed space of D." Let M be a fine Fourier space. Let $|g)$ be the Fourier transformation of $|f(x))$, $f(x) \in M$, and let $\langle\Phi|$ be the Fourier transformation of $\langle\psi|$, $\langle\psi| \in M^\dagger$. Then $\langle\psi\,|f(x))$ exists and we define $\langle\Phi|$ by

$$\langle\Phi\,|\,g) \equiv \langle\psi\,|f), \tag{2.51}$$

for all $|f)$ in M. Thus every $\langle\psi|$ in $M^\dagger$ has a Fourier transformation. Further, any series in the form

$$\sum_{n=-\infty}^{\infty} a_n \exp(inx),$$

whose coefficients increase no faster than some power of n as $n \to \infty$, can be put[6] in one-to-one correspondence with an element of $\mathfrak{W}$.

We have previously defined the functional $\langle\delta|$ by $\langle\delta\,|f(x)) \equiv f(0)$. Now we define a one-parameter class by $\langle\delta(k)\,|f(x)) \equiv f(k)$. The domain of $\langle\delta(k)|$ is all those functions $g(x)$, for which $g(k)$ is defined. If $g(x)$ is such a function, then $\langle\delta(k)\,|\,g(x)) \equiv g(k)$. When several variables, x, y, z, etc., are involved we write $\langle\delta(k-x)|$ to indicate that $\langle\delta(k)|$ is a functional on those functions considered as functions of x. We define $\langle a(x,k)\delta(k-x)|$ on the set of all $f(x)$ such that $\hat{D}_x^\alpha f(x)$ exists at $x = k$, and where $a(x,k)$ is a quasi-good function in x such that $\lim_{x\to k}(x-k)^\alpha a^*(x,k)$ is finite and α is the smallest nonnegative number for which it is finite, by

$$\langle a(x,k)\delta(k-x)\,|f(x)) \equiv \lim_{x\to k}[a^*(x,k)(x-k)^\alpha\Gamma^{-1}(\alpha+1)\hat{D}_x^\alpha f(x)], \tag{2.52}$$

where $\Gamma^{-1}(\alpha+1)$ refers to the inverse of the usual Γ function. $\hat{D}_x^\alpha$ is defined on all $f(x)$ for which the integral in (2.53) converges for $\alpha > 0$, by

$$\hat{D}_x^\alpha f(x) = \frac{1}{\Gamma(p)}\int_{-\infty}^{x}(x-t)^{p-1}\frac{d^m}{dt^m}f(t)\,dt, \tag{2.53}$$

where m is the least integer greater than α and $m - \alpha \equiv p$. Thus, $0 < p \leq 1$. If α is an integer, $\hat{D}_x^\alpha = d^\alpha/dx^\alpha$. The definition of $\hat{D}_x^\alpha$ is a slightly modified version of the usual definition of differentiation to fractional orders. Note that $\langle a(x,k)\delta(k-x)|$ is not a point function and that

$$\langle a(x,k)\delta(k-x)\,|f(x)) \neq \langle\delta(k-x)\,|\,a^*(x,k)f(x))$$

unless $a^*(x,k)$ is infinitely differentiable for all x. [See (2.6)]

D. Orthogonality and Multidimensional Spaces

If F, G, $\mathfrak{F}$, and $\mathfrak{G}$ are compatible sets, $\hat{A}$ is said to be an operator "upon" them if it maps $\mathfrak{F}$ into $\mathfrak{F}$ and $\mathfrak{G}$ into $\mathfrak{G}$. Let $\hat{A}$ be an operator acting to the right upon the compatible sets F, G, $\mathfrak{F}$, and $\mathfrak{G}$. That is, for every $|f\rangle$ in $\mathfrak{F}$ and $|g\rangle$ in $\mathfrak{G}$,

$$\hat{A}\,|f\rangle = |h_1\rangle; \quad \hat{A}\,|g\rangle = |h_2\rangle, \tag{2.54}$$

for some $|h_1\rangle$ in $\mathfrak{F}$ and $|h_2\rangle$ in $\mathfrak{G}$. We now define $'\hat{A}$ acting to the left on these compatible sets by

$$\langle g|\,\hat{A}\,|f) \equiv (g|\,\hat{A}\,|f\rangle \tag{2.55}$$

for all $\langle g|$ in $\mathfrak{G}^*$ and $|f\rangle$ in $\mathfrak{F}$.

It follows from (2.55) and (2.45) that $\hat{A}$ is Hermitian if and only if $\hat{A} = \hat{A}^*$.

Let $\mathfrak{F}$ be a self-compatible space and $\hat{A}$ an operator on it. Then if for some number β and some $|f\rangle$ in $\mathfrak{F}$

$$\hat{A}\,|f\rangle = \beta\,|f\rangle, \tag{2.56}$$

it follows from (2.55) that, since by (2.43) $(f\,|f\rangle$ is real,

$$\langle f|\,\hat{A}\,|f) = (f|\,\hat{A}\,|f\rangle = \beta(f\,|\,f\rangle = \beta\langle f\,|f). \tag{2.57}$$

Equation (2.57) implies that

$$\langle f|\,\hat{A} = \langle f|\,\beta + \langle h|, \tag{2.58}$$

where $\langle h|$ satisfies

$$\langle h\,|f) = 0. \tag{2.59}$$

We say that a set of kets $\{|f(n)\rangle\}$ in a self-compatible space are "orthogonal" if $(f(m)\,|f(n)\rangle = 0$, for $m \neq n$. If $|f(n)\rangle$ is an eigenket of $\hat{A}$ with eigenvalue $\beta(n)$, it follows from (2.58) that, for $n \neq m$,

$$\begin{aligned} 0 &= \beta(m)(f(n)\,|f(m)\rangle = (f(n)|\,\hat{A}\,|f(m)\rangle \\ &= \langle f(n)|\,\hat{A}\,|f(m)) \\ &= \beta(n)\langle f(n)\,|f(m)) + \langle h(n)\,|f(m)) = \langle h(n)\,|f(m)). \end{aligned} \tag{2.60}$$

But since (2.59) tells us that $\langle h(n)\,|f(n)) = 0$, $\langle h(n)|$ is orthogonal to every eigenfunction of $\hat{A}$. Thus if the eigenfunctions of $\hat{A}$ form a complete orthogonal set in $\mathfrak{F}$, $\langle h(n)| = 0$.

Let $\hat{B}$ be an operator on the self-compatible space $\mathfrak{F}$ whose eigenkets form a complete orthogonal set in

[6] W. Kaplan, *Advanced Calculus* (Addison-Wesley Publ. Co., Inc., Reading, Mass., 1952), pp. 357–358.

$\mathcal{F}$. Let $|f(n)\rangle$ be the eigenket of $\hat{B}$ with eigenvalue $\beta(n)$. Then if $\hat{A}$ is an operator with domain $\mathcal{G}$ which satisfies

$$[\hat{B}, \hat{A}] \equiv \hat{B}\hat{A} - \hat{A}\hat{B} = -i\hbar \tag{2.61}$$

on $\mathcal{F} \cap \mathcal{G}$, it follows that for $|f(m)\rangle$ and $|f(n)\rangle$ in $\mathcal{F} \cap \mathcal{G}$,

$$\begin{aligned} -i\hbar(f(m)\,|\,f(n)\rangle &= (f(m)|\,\hat{B}\hat{A} - \hat{A}\hat{B}\,|f(n)\rangle \\ &= (\beta(m) - \beta(n))(f(m)|\,\hat{A}\,|f(n)\rangle. \end{aligned} \tag{2.62}$$

Consider a linear functional $\langle F|$ defined on an appropriate set G of functions x and y. That is, $\langle F\,|\,f(x, y))$ is a complex number for every $|f(x, y))$ in G. Now consider a function of the form $|K(x, y)) = |f(x))\,|g(y))$. Then

$$\langle F\,|\,K(x, y)) = \langle F\,|\,f(x))\,|g(y)) \tag{2.63}$$

is a number. $\langle F\,|\,f(x))$, however, is a functional on the appropriate set of functions of y. Similarly, we define ${}_x\langle F\,|\,f(x)g(y))$ by

$${}_x\langle F\,|\,f(x)g(y))\,|h(y)) \equiv \langle F\,|\,f(x))\,|g(y)h(y)). \tag{2.64}$$

That is, if $\langle F\,|\,f(x)) = \langle E|$, where $\langle E|$ is a functional on the appropriate set of functions of y,

$${}_x\langle F\,|\,f(x)g(y)) = \langle g^*(y)E|. \tag{2.65}$$

For some general function $L(x, y)$ in the domain of $\langle F|$, we mean by ${}_x\langle F\,|\,L(x, y))$ that functional on the appropriate functions of y which is arrived at by considering y as a fixed parameter and calculating $\langle F\,|\,L(x, y))$ as if $L(x, y)$ were a function only of x.

For each n we can view $(f(m)\,|\,f(n)\rangle$ in (2.62) as a functional on a set of functions of the variable represented by m. In fact, we could write it $(f(x, m)\,|\,f, n\rangle_x$ where the f in the ket denotes the functional acting in x space [in this case the counterpart of $f(x)$] and the n denotes the functional acting in m space. By convention the order of variables in the function is made the same as the order of the indices in the functional acting on it, the index in the functional being in the same position as the variable acted upon. Thus for any $(j(m)|$ in the domain D of both $(f(x, m)\,|\,f, n\rangle_x$ and $(\beta(m) - \beta(n))(f(x, m)|\,\hat{A}\,|f, n\rangle_x$, we have

$$\begin{aligned} &i\hbar(j(m)|\,(f(x, m)\,|f, n\rangle_x\rangle_m \\ &= (j(m)|\,(\beta(m) - \beta(n))(f(x, m)|\,\hat{A}\,|f, n\rangle_x\rangle_m. \end{aligned} \tag{2.66}$$

A solution to (2.66) is

$$\begin{aligned} &(f(x, m)|\,\hat{A}\,|f, n\rangle_x \\ &\quad = i\hbar(\beta(m) - \beta(n))^{-1}(f(x, m)\,|f, n\rangle_x. \end{aligned} \tag{2.67}$$

It is unique in the sense that if $(k(m)\,|\,N\rangle_x$ is also a solution,

$$\begin{aligned} &(j(m)|\,[i\hbar(\beta(m) - \beta(n))^{-1}(f(x, m)\,|f, n\rangle_x \\ &\qquad - (k(m)\,|\,N\rangle_x]\rangle_m = 0 \end{aligned} \tag{2.68}$$

for all $(j(m)|$ in D.

Thus we have solved for the "matrix elements" of $\hat{A}$, that is, the linear functional on functions of m, $(f(x, m)|\,\hat{A}\,|f, n\rangle_x$. Note that no inherent restrictions (such as being in S) have been placed on the functions of m and that m itself might even take on only discrete values.

We consider one specific example. Assume that m is a continuous variable and that $\beta(m)$ takes on all values in a certain range. Then letting $|g(m))$ be the eigenket of $\hat{B}$ with eigenvalue m, Eq. (2.67) can be written, for m in this range,

$$(g(x, m)|\,\hat{A}\,|g, n\rangle_x = i\hbar(m - n)^{-1}(g(x, m)\,|\,g, n\rangle_x. \tag{2.69}$$

If, in addition,

$$\begin{aligned} &(m - n)^{-1}(g(x, m)\,|\,g, n\rangle_x \\ &\qquad = |(m - n)^{-1}\delta(n - m)\rangle, \end{aligned} \tag{2.70}$$

we get from (2.52) that, for all $(j(m)|$ with continuous first derivatives in a neighborhood of $m = n$,

$$\begin{aligned} &(j(m)|\,(g(x, m)|\,\hat{A}\,|g, n\rangle_x\rangle_m \\ &\qquad = i\hbar(j(m)|\,(m - n)^{-1}\delta(n - m)\rangle_m \\ &\qquad = i\hbar\frac{d}{dn}\,|j^*(n)). \end{aligned} \tag{2.71}$$

The unique solution to (2.71) is

$$(g(x, m)|\,\hat{A}\,|g, n\rangle_x = i\hbar\frac{d}{dm}\,|\delta(n - m)\rangle. \tag{2.72}$$

Canonically conjugate operators play a fundamental role in this development of quantum mechanics. In the following section we show how, given two canonically conjugate operators $\hat{q}$ and $\hat{p}$ (not necessarily space and momentum), one can find the canonical conjugate of any function of these operators if the canonical conjugate exists and is "expandable," that is, can be written in the form

$$\sum_{j=-\infty}^{\infty} a_{ij}\hat{q}^i\hat{p}^j \quad (a_{ij} = \text{const, all } i, j).$$

E. Representable Operators

Consider an operator $\hat{A}$, defined for all $|\psi\rangle$ in its domain $\mathcal{D}(\hat{A})$ by

$$\hat{A}\,|\psi\rangle = |\Phi(\psi)\rangle. \tag{2.73}$$

We can define a function $(g|$ by demanding that, for every $(f|$ in $\mathfrak{D}(\mathfrak{R}(\hat{A}))$,

$$(g \mid \psi\rangle = (f \mid \Phi(\psi)\rangle = (f \mid \hat{A} \mid \psi\rangle, \qquad (2.74)$$

where $\mathfrak{R}(\hat{A})$ is the range of $\hat{A}$. If such a $(g|$ exists for each $(f|$, it is unique and we call $\hat{A}$ a "representable" operator.

If $\hat{A}$ is a representable operator, we can define its action on every $(f|$ in $\mathfrak{D}(\mathfrak{R}(\hat{A}))$ by

$$(g| \equiv (f| \hat{A}. \qquad (2.75)$$

Similarly the complex conjugate of (2.74) implies

$$\hat{A}^* |f) = |g). \qquad (2.76)$$

It follows that we can define a representable operator $\hat{A}$ by specifying a linear mapping (also denoted by $\hat{A}$) from $\mathfrak{D}(\mathfrak{R}(\hat{A}))$ into $\mathfrak{D}(\mathfrak{D}(\hat{A}))$. Such a specification of a representable operator $\hat{A}$ is called a "representation" of $\hat{A}$. For example, (2.16) and (2.17) define $\hat{x}$ and $\hat{p}$ in terms of representations.

3. EQUATIONS FOR THE CANONICAL CONJUGATE OF AN ARBITRARY OPERATOR

The domain of $\hat{q}^{-1}$ consists of all those generalized functions whose domain includes $(g/x|$ for all $(g|$ in S^*. We define $\hat{q}^{-1}$ on this domain by $\hat{q}^{-1} |f) = |x^{-1}f)$, where $|x^{-1}f)$ is defined by $(g \mid x^{-1}f) \equiv (x^{-1}g \mid f)$ for all g in $\mathfrak{D}(|x^{-1}f))$.

$\hat{p}^{-1}$ is defined on all of $\mathfrak{W}^*$ by $\hat{p}^{-1} |f\rangle = |p^{-1}f\rangle$, where $|p^{-1}f\rangle$ is defined on all $(g|$ such that

$$\left(\int_{-\infty}^{x} dy g(y)\right| \quad \text{is in} \quad \mathfrak{D}(|f))$$

by

$$(g \mid p^{-1}f\rangle \equiv \left(\frac{i}{\hbar}\int_{-\infty}^{x} dy g(y) \,\middle|\, f\right\rangle.$$

Since if $(g| \in S^*$,

$$\left(\int_{-\infty}^{x} dy g(y)\right| \in S^*, \quad \text{then} \quad \mathfrak{D}(|p^{-1}f)) \supseteq S.$$

It is easy to prove that $|p^{-1}f\rangle$ is linear. What is more, since, for any sequence of good functions $\{g_n(y)\}$, if $\{g_n(y)\}$ converges to zero,

$$\left\{\int_{-\infty}^{x} dy g_n(y)\right\}$$

converges to zero, then $|p^{-1}f\rangle$ is continuous.

It follows from the above definitions that

$$\hat{p}^{-1}\hat{p} = \hat{p}\hat{p}^{-1} = \hat{I},$$

where $\hat{I}$ is the identity operator for all of $\mathfrak{W}^*$. It also follows that

$$\hat{x}^{-1}\hat{x} = \hat{x}\hat{x}^{-1} = \hat{I}(\hat{x}^{-1}),$$

where $\hat{I}(\hat{x}^{-1})$ is the identity operator for $\mathfrak{D}(\hat{x}^{-1})$.

In the following the formulas are true, of course, only insofar as the functional acted upon is in the domain of the operators concerned.

In a previous paper[7] we have shown that if $\hat{q}$ and $\hat{p}$ obey $[\hat{p}, \hat{q}] = -i\hbar$, for any integers α and β, positive or negative,

$$\begin{aligned}[\hat{p}^{\alpha}, \hat{q}^{\beta}] = {} & (1 - \delta_{\alpha,0})(1 - \delta_{\beta,0}) \\ & \times \sum_{m=1}^{\Omega(\alpha,\beta)} \binom{|\alpha| + (m-1)\theta(-\alpha)}{m} \\ & \times \binom{|\beta| + (m-1)\theta(-\beta)}{m} \\ & \times (i\hbar)^m (-1)^{\sigma(\alpha,\beta)m} m!\, \hat{q}^{\beta-m}\hat{p}^{\alpha-m}, \end{aligned} \qquad (3.1)$$

where $\binom{a}{b}$ is the binomial coefficient, $a!/b!\,(a-b)!$

$$\begin{aligned} \theta(q) &\equiv 0, \quad \text{for} \quad q < 0, \\ &\equiv 1, \quad \text{for} \quad q \geq 0; \end{aligned}$$

$\sigma(\alpha, \beta) \equiv 1$, when α and β have the same sign,
$\equiv 0$, when α and β have different signs;

$\Omega(\alpha, \beta) \equiv$ the smaller of the two, if both α and β are positive,
$\equiv$ the positive one, if α and β are of different signs,
$\equiv +\infty$, if α and β are both negative.

It should be emphasized that (3.1) is an operator relationship and that there is no question of the convergence of the series on the right until the matrix elements of the operator have been formed.

We can now attack the problem of finding the canonical conjugate of any given operator if it exists and is expandable. If $\hat{F}(\hat{q}, \hat{p})$ and $\hat{G}(\hat{q}, \hat{p})$ are operator functions of $\hat{q}$ and $\hat{p}$ and if

$$[\hat{F}(\hat{q}, \hat{p}), \hat{G}(\hat{q}, \hat{p})] = -i\hbar, \qquad (3.2)$$

then $\hat{F}(\hat{q}, \hat{p})$ and $\hat{G}(\hat{q}, \hat{p})$ are called "canonical conjugates." Consider a function $\hat{F}(\hat{q}, \hat{p})$ in the form

$$\hat{F}(\hat{q} \mid \hat{p}) = \sum_{k=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} a_{kn}\hat{q}^k\hat{p}^n. \qquad (3.3)$$

An operator function $\hat{F}$ of $\hat{q}$ and $\hat{p}$ with the $\hat{p}$'s to the right of the $\hat{q}$'s in each term is said to be in "normal form" and will be written $\hat{F}(\hat{q} \mid \hat{p})$.

We ask for the set of all canonically conjugate $\hat{G}(\hat{q}, \hat{p})$ in the form

$$\hat{G}(\hat{q} \mid \hat{p}) = \sum_{\gamma=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} b_{\gamma j}\hat{q}^{\gamma}\hat{p}^{j}. \qquad (3.4)$$

Thus we require

$$\sum_{\gamma,j,k,n=-\infty}^{\infty} a_{kn}b_{\gamma j}[\hat{q}^k\hat{p}^n, \hat{q}^{\gamma}\hat{p}^{j}] = -i\hbar.$$

[7] D. M. Rosenbaum, J. Math. Phys. **8**, 1973 (1967).

This leads easily to

$$\sum_{\gamma,j,k,n=-\infty}^{\infty}(a_{kn}b_{\gamma j}-a_{\gamma j}b_{kn})\hat{q}^k[\hat{p}^n,\hat{q}^\gamma]\hat{p}^j=-i\hbar. \quad (3.5)$$

Putting $[\hat{p}^n,\hat{q}^\gamma]$ into (3.5) from (3.1), we get

$$\sum_{\gamma,j,k,n=-\infty}^{\infty}(1-\delta_{n,0})(1-\delta_{\gamma,0})(a_{kn}b_{\gamma j}-a_{\gamma j}b_{kn})$$
$$\times\sum_{m=1}^{\Omega(n,\gamma)}\binom{|n|+(m-1)\theta(-n)}{m}\binom{|\gamma|+(m-1)\theta(-\gamma)}{m}$$
$$\times(i\hbar)^m(-1)^{\sigma(n,\gamma)m}m!\,\hat{q}^{\gamma+k-m}\hat{p}^{j+n-m}=-i\hbar. \quad (3.6)$$

This can be rewritten as

$$\sum_{\alpha,\beta=-\infty}^{\infty}\sum_{\gamma,n=-\infty}^{\infty}(1-\delta_{n,0})(1-\delta_{\gamma,0})$$
$$\times\sum_{m=1}^{\Omega(n,\gamma)}\alpha_{\beta+m-\gamma,n}b_{\gamma,\alpha+m-n}-a_{\gamma,\alpha+m-n}b_{\beta+m-\gamma,n}$$
$$\times\binom{|n|+(m-1)\theta(-n)}{m}\binom{|\gamma|+(m-1)\theta(-\gamma)}{m}$$
$$\times(i\hbar)^m(-1)^{\sigma(n,\gamma)m}m!\,\hat{q}^\beta\hat{p}^\alpha=-i\hbar. \quad (3.7)$$

Equating the coefficients of $\hat{q}^\beta\hat{p}^\alpha$ on each side of (3.7), we get

$$\sum_{\gamma,n=-\infty}^{\infty}(1-\delta_{n,0})(1-\delta_{\gamma,0})$$
$$\times\sum_{m=1}^{\Omega(n,\gamma)}(a_{\beta+m-\gamma,n}b_{\gamma,\alpha+m-n}-a_{\gamma,\alpha+m-n}b_{\beta+m-\gamma,n})$$
$$\times\binom{|n|+(m-1)\theta(-n)}{m}\binom{|\gamma|+(m-1)\theta(-\gamma)}{m}$$
$$\times(i\hbar)^m(-1)^{\sigma(n,\gamma)m}m!=-i\hbar\delta_{\alpha,0}\delta_{\beta,0}. \quad (3.8)$$

For a given set of coefficients a_{kn}, Eq. (3.8) determines the coefficients b_{ij}. When an infinite homogeneous linear set of indicial equations determines an infinite set of two-indexed coefficients, as in (3.8), there are in general an infinite set of arbitrary constants undetermined. The above procedure gives the most general canonical conjugate.

In general, we insist that $\hat{G}(\hat{p}\,|\,\hat{q})$ be Hermitian. This can always be done if $\hat{F}$ is Hermitian, since then the adjoint of (3.2) is

$$[\hat{F},\hat{G}^*]=-i\hbar. \quad (3.9)$$

From (3.2) and (3.9) it follows that $\frac{1}{2}(\hat{G}+\hat{G}^*)$ is a Hermitian operator which is canonically conjugate to F. We wish to have this operator in normal form, however. From (3.4), we have

$$\hat{G}^*=\sum_{\gamma=-\infty}^{\infty}\sum_{j=-\infty}^{\infty}b^*_{\gamma j}\hat{p}^j\hat{q}^\gamma=\sum_{\gamma,j=-\infty}^{\infty}b^*_{\gamma j}\{\hat{q}^\gamma\hat{p}^j+[\hat{p}^j,\hat{q}^\gamma]\}=\sum_{\gamma,j=-\infty}^{\infty}b^*_{\gamma j}\Big\{\hat{q}^\gamma\hat{p}^j+(1-\delta_{j,0})(1-\delta_{\gamma,0})$$
$$\times\sum_{m=1}^{\Omega(\gamma,j)}\binom{|\gamma|+(m-1)\theta(-\gamma)}{m}\binom{|j|+(m-1)\theta(-j)}{m}(i\hbar)^m(-1)^{\sigma(\gamma,j)m}m!\,\hat{q}^{\gamma-m}\hat{p}^{j-m}\Big\}$$
$$=\sum_{\gamma,j=-\infty}^{\infty}b^*_{\gamma j}\Big\{1+(1-\delta_{\gamma,-1})(1-\delta_{j,-1})\sum_{m=1}^{v(\gamma,j)}(1-\delta_{m,-\gamma})(1-\delta_{m,-j})\binom{|m+\gamma|+(m-1)\theta(-m-\gamma)}{m}$$
$$\times\binom{|m+j|+(m-1)\theta(-m-j)}{m}(i\hbar)^m(-1)^{\sigma(m+\gamma,m+j)}m!\Big\}\hat{q}^\gamma\hat{p}^j, \quad (3.10)$$

where

$$\begin{aligned}v(\gamma,j)&\equiv\infty, && \text{if } \gamma\geq 0 \text{ and } j\geq 0,\\ &\equiv -\gamma-1, && \text{if } \gamma\leq -2 \text{ and } j\geq 0,\\ &\equiv -j-1, && \text{if } \gamma\geq 0 \text{ and } j\leq -2,\\ &\equiv \text{the smaller of } (-\gamma-1) \text{ and } (-j-1), && \text{if } \gamma\leq -2 \text{ and } j\leq -2.\end{aligned}$$

In the next two sections we discuss the time operator, the canonical conjugate of the Hamiltonian.

4. CLASSICAL CANONICAL TIME

We write the Poisson bracket of two variables A and B as $\{A,B\}$. If q and p are canonically conjugate variables, then

$$\{q,p\}=1. \quad (4.1)$$

For a given Hamiltonian $H(q,p)$, we search for $T(q,p)$, such that

$$\{T,H\}=1. \quad (4.2)$$

The change in any $U(q,p)$ under an infinitesimal canonical transformation generated by T is, for infinitesimal ϵ,

$$\delta U=\epsilon\{U,T\}. \quad (4.3)$$

For $\epsilon=-dE$, $U=H$, we get

$$\delta H=dE, \quad (4.4)$$

and integrating we get

$$H=H_0+E. \quad (4.5)$$

Thus $T(q, p)$ is the generator of energy transformations in just the same way that $H(q, p)$ is the generator of the system's motion in time. Just as quantities whose Poisson bracket with H vanishes are constant in time, quantities whose Poisson bracket with T vanishes are constant under changes in energy.

From (4.3) we also find

$$\delta p = dE\{p, T\} = dE\frac{\partial T}{\partial q}, \tag{4.6}$$

$$\delta q = dE\{q, T\} = -dE\frac{\partial T}{\partial p}. \tag{4.7}$$

A. The Free Particle

For a free particle, (4.2) is just

$$\frac{\partial T}{\partial q}\frac{p}{m} = 1, \tag{4.8}$$

which gives

$$T(q, p) = (m/p)q + f(p) \tag{4.9}$$

where $f(p)$ is an arbitrary function of p. This can be written

$$q = (p/m)T - pf(p)/m. \tag{4.10}$$

If, for some constant $q(0)$, we pick

$$f(p) = -(m/p)q(0), \tag{4.11}$$

then (4.10) becomes

$$q = (p/m)T + q(0). \tag{4.12}$$

Thus one of the possible canonically conjugate $T(q, p)$ is just $t(q, p)$, the inverted solution to the dynamical equations. This is true for any Hamiltonian since, $T(q, p)$ not being an explicit function of time,

$$\frac{dT}{dt} = \{T, H\} + \frac{\partial T}{\partial t} = 1. \tag{4.13}$$

Thus T can differ from $t(q, p)$ at most by a constant. Finding $T(q, p)$ for an $H(q, p)$ is, in effect, a solution of the dynamical equations of motion for the system represented by that $H(q, p)$ and can be used as a method for solving such equations.

From (4.9) and (4.6),

$$\delta p = dE(m/p), \tag{4.14}$$

or

$$\frac{1}{2m}\int_{p_0^2}^{p^2} d(p^2) = \int_{E_0}^{E} dE. \tag{4.15}$$

If $p_0^2/(2m) = E_0$, then (4.15) gives

$$E = p^2/(2m). \tag{4.16}$$

Thus, if T generates a change E in the energy, it changes p just enough to keep (4.16) true. From (4.12) and (4.7),

$$\delta q = dE(mq/(p^2) - df/dp). \tag{4.17}$$

If we choose $f(p)$ as in (4.11), (4.17) integrates to give

$$q = q_0(p - p_0)/p_0. \tag{4.18}$$

B. The Harmonic Oscillator

We will not go through the derivation of the analogous results for the harmonic oscillator, but simply state them. For $\omega = (k/m)^{\frac{1}{2}}$, $V = \frac{1}{2}kq^2$, $K = (p^2/2m)$,

$$T = (1/\omega)\tan^{-1}(V/K)^{\frac{1}{2}}, \tag{4.19}$$

$$p = p_0(E/E_0)^{\frac{1}{2}}; \quad q = q_0(E/E_0)^{\frac{1}{2}}. \tag{4.20}$$

Once again, since $E_0 = (p_0^2/2m) + \frac{1}{2}kq_0^2$,

$$E = (p^2/2m) + \tfrac{1}{2}kq^2.$$

Note that T is just the dynamical time t and that time is cyclic; i.e., unless one can count cycles, only the phase is meaningful.

These classical results constitute the boundary values for the corresponding quantum-mechanical problems via the correspondence principle.

5. QUANTUM-MECHANICAL TIME OPERATOR

We define the time operator $\hat{T}$ by

$$[\hat{H}, \hat{T}] = -i\hbar. \tag{5.1}$$

$\hat{T}$ is a function of $\hat{q}$ and $\hat{p}$ and never depends explicitly on time unless $\hat{H}$ does. It follows from (5.1) and the Heisenberg equations of motion that if $\hat{T}$ is considered as a Heisenberg operator $\hat{T}_0$ and does not depend explicitly on time, then

$$\frac{d\hat{T}_0}{dt} = 1. \tag{5.2}$$

If (5.1) and (5.2) are true for the Heisenberg operator $\hat{T}_0$, they are also true for the Schrödinger operator $\hat{T} \equiv \exp(i\hat{H}t/\hbar)\hat{T}_0\exp(-i\hat{H}t/\hbar)$, assuming that it exists.

The eigenvalue t of $\hat{T}$ is just the parameter time which appears in the Hilbert-space formulation of quantum mechanics. If we measure the energy of a particle exactly, we force it into an energy eigenstate whose eigenvalue is the measured energy; if we measure when a particle experiences an event, we force it into a time eigenstate whose eigenvalue is the measured time.

Now we consider some specific $\hat{T}$'s. For any given $\hat{H}$, Eq. (3.8) can be explicitly solved for $\hat{T}$ just by methodically solving the equations.

A. The Free Particle

In order to illustrate the method of solving (3.8) we derive the solution for the free particle in detail. For the free particle $\hat{H} = \hat{p}^2/2m$, and the coefficients a_{ke} in (3.3) are

$$a_{ke} = (2m)^{-1}\,\delta_{k,0}\delta_{e,2}. \tag{5.3}$$

Equation (3.8) then becomes

$$\sum_{i=-\infty}^{\infty}(1-\delta_{i,0})\sum_{n=1}^{\tau(2,i)}\delta_{n,i-\beta}b_{i,\alpha+n-2}\binom{2}{n} \times \binom{|i|+(n-1)\theta(-i)}{n}(i\hbar)^n(-1)^{\sigma(2,i)n}n! = -2i\hbar m\delta_{\alpha,0}\delta_{\beta,0}. \tag{5.4}$$

Splitting the sum over i into three pieces, we get

$$\sum_{n=1}^{2}\left\{\sum_{i=-\infty}^{-1}\delta_{i,n+\beta}b_{i,\alpha+n-2}\binom{2}{n}(i\hbar)^n n!\binom{n-1-i}{n} + \sum_{i=2}^{\infty}\delta_{i,n+\beta}b_{i,\alpha+n-2}\binom{2}{n}\binom{i}{n}(-i\hbar)^n n!\right\} - 2i\hbar\delta_{\beta,0}b_{1,\alpha-1} = -2mi\hbar\delta_{\alpha,0}\delta_{\beta,0}. \tag{5.5}$$

Recall that

$$\theta(x) = 1, \quad x \geq 0, \qquad = 0, \quad x < 0. \tag{5.6}$$

Then (5.5) becomes

$$\sum_{n=1}^{2}\left\{\theta(-1-n-\beta)b_{n+\beta,n+\alpha-2}\binom{2}{n}\binom{-1-\beta}{n}(i\hbar)^n n! + \theta(n+\beta-2)b_{n+\beta,n+\alpha-2}\binom{2}{n}\binom{n+\beta}{n}(-i\hbar)^n n!\right\} - 2i\hbar\delta_{\beta,0}b_{1,\alpha-1} = -2i\hbar m\delta_{\alpha,0}\delta_{\beta,0}. \tag{5.7}$$

Doing out the sum over n, we get

$$(\beta+1)b_{\beta+1,\alpha-1}(\theta(\beta-1)+\theta(-\beta-2)) - [\tfrac{1}{2}(\beta+1)(\beta+2)]i\hbar b_{\beta+2,\alpha}(\theta(\beta)+\theta(-\beta-3)) + \delta_{\beta,0}b_{1,\alpha-1} = m\delta_{\alpha,0}\delta_{\beta,0}. \tag{5.8}$$

Equation (5.8) can be written as

$$(\beta+1)b_{\beta+1,\alpha-1} - [\tfrac{1}{2}(\beta+1)(\beta+2)](i\hbar)b_{\beta+2,\alpha} = m\delta_{\alpha,0}\delta_{\beta,0}. \tag{5.9}$$

The choice $\beta = 0$ gives

$$b_{2,\alpha} = (i\hbar)^{-1}(b_{1,\alpha-1} - m\delta_{\alpha,0}). \tag{5.10}$$

The choice $\beta = -1$ gives nothing and $\beta = -2$ gives

$$b_{-1,\alpha} = 0. \tag{5.11}$$

Lastly, we get

$$b_{\beta+1,\alpha+1} = \left(\frac{2}{i\hbar}\right)\frac{1}{\beta+1}\,b_{\beta,\alpha} \quad (\beta \neq 1, 0, -1). \tag{5.12}$$

Equation (5.11) and (5.12) together lead immediately to

$$b_{\beta,\alpha} = 0 \quad (\beta < 0). \tag{5.13}$$

The determining set of Eqs. (5.10)–(5.12) leaves the $b_{0,\alpha}$'s and $b_{1,\alpha}$'s arbitrary but gives, through (5.10) and (5.12), the $b_{\beta,\alpha}$'s ($\beta \geq 2$) in terms of these. Thus we get

$$b_{j,k} = \left(\frac{2}{i\hbar}\right)^{j-1}\frac{1}{j!}(b_{1,k+1-j} - m\delta_{k,j-2}) \quad (j \geq 2). \tag{5.14}$$

Thus the time operator for a free particle has the form

$$\hat{T} = \sum_{k=-\infty}^{\infty}\left\{b_{0,k} + b_{1,k}\hat{q} + \sum_{j=2}^{\infty}\left(\frac{2}{-i\hbar}\right)^{j-1}\frac{1}{j!}(b_{1,k+1-j} - m\delta_{k,j-2})\hat{q}^j\right\}\hat{p}^k, \tag{5.15}$$

where the $b_{0,k}$'s and $b_{1,k}$'s are arbitrary. Since the coefficients of $\hat{q}^j$ for $j \geq 2$ depend explicitly on inverse powers of $\hbar$, we cannot pass to the classical limit by letting $\hbar \to 0$ unless these coefficients are all zero. This can be done by setting

$$b_{1,\beta} = m\delta_{\beta,-1}, \tag{5.16}$$

for all β. This gives

$$\hat{T} = \sum_{k=-\infty}^{\infty} b_{0,k}\hat{p}^k + m\hat{q}\hat{p}^{-1}. \tag{5.17}$$

As $\hat{q}$ and $\hat{p}$ commute classically, the different possible forms in which an operator $\hat{A}(\hat{p}, \hat{q})$ can be put using the commutation rules give different classical limits. We call the form $\frac{1}{2}[\hat{A}(\hat{q}\,|\,\hat{p}) + \hat{A}(\hat{p}\,|\,\hat{q})]$ the "manifestly Hermitian form" of $\hat{A}(\hat{p}, \hat{q})$. We now make the rule that an operator must be put in this form before the classical limit is taken. Thus putting $\hat{T}$ in this form we get [the $b_{0,k}$ here are different from those in (5.17)],

$$\hat{T} = \sum_{k=-\infty}^{\infty} b_{0,k}\hat{p}^k + \tfrac{1}{2}m(\hat{q}\hat{p}^{-1} + \hat{p}^{-1}\hat{q}). \tag{5.18}$$

Then for $\hat{T}$ to approach the classical t as $\hbar \to 0$, we must have

$$b_{0,k} \xrightarrow[\hbar\to 0]{} -mq_0\delta_{k,-1}, \tag{5.19}$$

where q_0 is an arbitrary constant. Then in the classical limit we get

$$t = -mq_0p^{-1} + mqp^{-1}. \tag{5.20}$$

Inverting (5.20) we get

$$q = q_0 + vt. \tag{5.21}$$

It is often convenient to set all the $b_{0,k} = 0$ and consider $\hat{T}$ as just

$$\hat{T} = \tfrac{1}{2}m(\hat{q}\hat{p}^{-1} + \hat{p}^{-1}\hat{q}). \tag{5.22}$$

Note that the domain of the $\hat{T}$ given in (5.22) is all of $\mathfrak{W}^*$.

The eigenkets of T cannot be expressed as functionals on functions of x. The eigenkets of $\hat{T}$ are functionals on functions of space–time, the eigenket with eigenvalue t_0 being $|\delta(t_0 - t)\rangle$.

B. The Harmonic Oscillator

As in the classical harmonic-oscillator example, we do not go through the derivation, but merely display a result. For reasons of space and because a following paper is planned giving the complete time operator for the harmonic oscillator and some of its uses, we give here only a particular solution for the time operator. To this must be added the most general operator function which commutes with the Hamiltonian. The constants must then be fixed so that $\hat{T}$ approaches the classical T as $\hbar \to 0$.

We display a $\hat{T}$ of the form

$$\hat{T} = \sum_{\alpha=2}^{\infty} \sum_{\beta=0}^{\infty} b_{\alpha,\beta} \hat{q}^{\alpha} \hat{p}^{\beta}, \tag{5.23}$$

such that

$$[\hat{H}, \hat{T}] = -i\hbar. \tag{5.24}$$

If we define

$$G \equiv \frac{-i\hbar}{2}; \quad K \equiv mk, \tag{5.25}$$

then (5.24) becomes

$$\frac{K}{2m}[\hat{q}, \hat{T}] + \frac{1}{2m}[\hat{p}^2, \hat{T}] = 2G. \tag{5.26}$$

Let $B(x)$ be the largest integer which is less than or equal to x. Then $b_{\alpha,\beta}$ can be written in the form

$$b_{\alpha,\beta} = -\frac{m}{\alpha!} \sum_{n=0}^{B[(\alpha-2)/4]} \frac{K^n}{G^{(\alpha-2n-1)}} C_{\alpha,n} \delta_{\beta,\alpha-2-4n}. \tag{5.27}$$

This gives

$$\hat{T} = -\sum_{\alpha=2}^{\infty} \frac{m}{\alpha!} \sum_{n=0}^{B[(\alpha-2)/4]} \frac{K^n}{G^{(\alpha-2n-1)}} C_{\alpha,n} \hat{q}^{\alpha} \hat{p}^{\alpha-2-4n}. \tag{5.28}$$

Consider $K/2m[\hat{q}^2, \hat{T}]$:

$$\frac{K}{2m}[\hat{q}^2, \hat{T}] = \frac{1}{2} \sum_{\alpha=2}^{\infty} \frac{1}{\alpha!} \sum_{n=0}^{B[(\alpha-2)/4]} \frac{K^{(n+1)}}{G^{(\alpha-2n-1)}} C_{\alpha,n} \hat{q}^{\alpha} [\hat{p}^{\alpha-2-4n}, \hat{q}^2]. \tag{5.29}$$

But

$$[\hat{p}^{\alpha-2-4n}, \hat{q}^2] = (1 - \delta_{\alpha,4n+2}) \sum_{m=1}^{L(\alpha-2-4n,2)} \binom{\alpha - 2 - 4n}{m} \binom{2}{m} (-2G)^m m!\, \hat{q}^{2-m} \hat{p}^{\alpha-2-4n-m}, \tag{5.30}$$

where $L(x, y)$ is equal to x or y, whichever is least. Thus

$$\begin{aligned}
\frac{K}{2m}[\hat{q}^2, \hat{T}] &= -\sum_{\alpha=2}^{\infty} \frac{2}{\alpha!} \sum_{n=0}^{B[(\alpha-3)/4]} \frac{K^{(n+1)}}{G^{(\alpha-2n-2)}} C_{\alpha,n} \delta_{\alpha,4n+3} \hat{q}^{\alpha+1} \\
&\quad + \frac{1}{2} \sum_{\alpha=2}^{\infty} \frac{1}{\alpha!} \sum_{n=0}^{B[(\alpha-4)/4]} \frac{K^{(n+1)}}{G^{(\alpha-2n-1)}} C_{\alpha,n} \sum_{m=1}^{2} \binom{\alpha - 2 - 4n}{m} \binom{2}{m} (-2G)^m m!\, \hat{q}^{\alpha+2-m} \hat{p}^{\alpha-2-4n-m} \\
&= -\sum_{n=0}^{\infty} \frac{2}{(4n+3)!} \frac{K^{(n+1)}}{G^{(2n+1)}} C_{4n+3,n} \hat{q}^{4(n+1)} - \sum_{\alpha=2}^{\infty} \frac{2}{\alpha!} \sum_{n=0}^{B[(\alpha-4)/4]} \frac{K^{(n+1)}}{G^{(\alpha-2n-2)}} (\alpha - 2 - 4n) C_{\alpha,n} \hat{q}^{\alpha+1} \hat{p}^{\alpha-3-4n} \\
&\quad + \sum_{\alpha=2}^{\infty} \frac{2}{\alpha!} \sum_{n=0}^{B[(\alpha-4)/4]} \frac{K^{(n+1)}}{G^{(\alpha-2n-3)}} (\alpha - 2 - 4n)(\alpha - 3 - 4n) C_{\alpha,n} \hat{q}^{\alpha} \hat{p}^{\alpha-4(n+1)}.
\end{aligned} \tag{5.31}$$

By changing the summation indices in (5.31), we can write it in the form

$$\begin{aligned}
\frac{K}{2m}[\hat{q}^2, \hat{T}] &= -\sum_{z=1}^{\infty} \frac{2}{(4z-1)!} \frac{K^z}{G^{(2z-1)}} C_{4z-1,z-1} \hat{q}^{4z} \\
&\quad - \sum_{\alpha=3}^{\infty} \frac{2}{(\alpha-1)!} \sum_{n=1}^{B[(\alpha-1)/4]} \frac{K^n}{G^{(\alpha-2n-1)}} (\alpha - 4n + 1) C_{\alpha-1,n-1} \hat{q}^{\alpha} \hat{p}^{\alpha-4n} \\
&\quad + \sum_{\alpha=2}^{\infty} \frac{2}{\alpha!} \sum_{n=1}^{B(\alpha/4)} \frac{K^n}{G^{(\alpha-2n-1)}} (\alpha - 4n + 2)(\alpha - 4n + 1) C_{\alpha,n-1} \hat{q}^{\alpha} \hat{p}^{\alpha-4n} \\
&= \sum_{\alpha=2}^{\infty} \frac{2}{\alpha!} \sum_{n=1}^{B(\alpha/4)} \frac{K^n}{G^{(\alpha-2n-1)}} (\alpha - 4n + 2)(\alpha - 4n + 1) C_{\alpha,n-1} \hat{q}^{\alpha} \hat{p}^{\alpha-4n} \\
&\quad - \sum_{\alpha=3}^{\infty} \frac{2}{(\alpha-1)!} \sum_{n=1}^{B(\alpha/4)} \frac{K^n}{G^{(\alpha-2n-1)}} (\alpha - 4n + 1) C_{\alpha-1,n-1} \hat{q}^{\alpha} \hat{p}^{\alpha-4n}.
\end{aligned} \tag{5.32}$$

Consider $1/(2m)[\hat{p}^2, \hat{T}]$:

$$\frac{1}{2m}[p^2, \hat{T}] = -\frac{1}{2}\sum_{\alpha=2}^{\infty}\frac{1}{\alpha!}\sum_{n=0}^{B[(\alpha-2)/4]}\frac{K^n}{G^{(\alpha-2n-1)}}C_{\alpha,n}[\hat{p}^2, \hat{q}^\alpha]\hat{p}^{\alpha-2-4n}. \tag{5.33}$$

But

$$[\hat{p}^2, \hat{q}^\alpha] = \sum_{m=1}^{2}\binom{\alpha}{m}\binom{2}{m}(-2G)^m m!\,\hat{q}^{\alpha-m}\hat{p}^{2-m}. \tag{5.34}$$

Thus

$$\frac{1}{2m}[\hat{p}^2, \hat{T}] = -\sum_{\alpha=2}^{\infty}\frac{2}{(\alpha-1)!}\sum_{n=0}^{B[(\alpha-2)/4]}\frac{K^n}{G^{(\alpha-2n-2)}}C_{\alpha,n}\hat{q}^{(\alpha-1)}\hat{p}^{\alpha-4n-1}$$

$$+\sum_{\alpha=2}^{\infty}\frac{2}{(\alpha-2)!}\sum_{n=0}^{B([\alpha-2)/4]}\frac{K^n}{G^{(\alpha-2n-3)}}C_{\alpha,n}\hat{q}^{(\alpha-2)}\hat{p}^{(\alpha-4n-2)} \tag{5.35}$$

$$= -\sum_{\alpha=1}^{\infty}\frac{2}{\alpha!}\sum_{n=0}^{B[(\alpha-1)/4]}\frac{K^n}{G^{(\alpha-2n-1)}}C_{\alpha+1,n}\hat{q}^\alpha\hat{p}^{\alpha-4n} + \sum_{\alpha=0}^{\infty}\frac{2}{\alpha!}\sum_{n=0}^{B(\alpha/4)}\frac{K^n}{G^{(\alpha-2n-1)}}C_{\alpha+2,n}\hat{q}^\alpha\hat{p}^{\alpha-4n}. \tag{5.36}$$

Thus

$$[H, \hat{T}] = \sum_{\alpha=0}^{\infty}\frac{2}{\alpha!}\sum_{n=0}^{B(\alpha/4)}\frac{K^n}{G^{(\alpha-2n-1)}}C_{\alpha+2,n}\hat{q}^\alpha\hat{p}^{\alpha-4n} - \sum_{\alpha=1}^{\infty}\frac{2}{\alpha!}\sum_{n=0}^{B[(\alpha-1)/4]}\frac{K^n}{G^{(\alpha-2n-1)}}C_{\alpha+1,n}\hat{q}^\alpha\hat{p}^{\alpha-4n}$$

$$-\sum_{\alpha=2}^{\infty}\frac{2}{\alpha!}\sum_{n=1}^{B(\alpha/4)}\frac{K^n}{G^{(\alpha-2n-1)}}(\alpha-4n+2)(\alpha-4n+1)C_{\alpha,n-1}\hat{q}^\alpha\hat{p}^{\alpha-4n}$$

$$+\sum_{\alpha=3}^{\infty}\frac{2}{(\alpha-1)!}\sum_{n=1}^{B(\alpha/4)}\frac{K^n}{G^{(\alpha-2n-1)}}(\alpha-4n+1)C_{\alpha-1,n-1}\hat{q}^\alpha\hat{p}^{\alpha-4n}. \tag{5.37}$$

If we set $C_{n,0} = 1$ for all n, the $\alpha = 0$ term gives $2G$ and the $\alpha = 1$, 2, and 3 terms equal zero. The $n = 0$ term equals zero for all α and (5.37) becomes

$$\sum_{\alpha=4}^{\infty}\frac{2}{\alpha!}\sum_{n=0}^{B[(\alpha-1)/4]}\frac{K^n}{G^{(\alpha-2n-1)}}\{C_{\alpha+2,n} - C_{\alpha+1,n} + (\alpha-4n+1)[\alpha C_{\alpha-1,n-1} - (\alpha-4n+2)C_{\alpha,n-1}]\}\hat{q}^\alpha\hat{p}^{\alpha-4n} = 0, \tag{5.38}$$

for $n < \alpha/4$, and for $n = \alpha/4$ we get

$$\sum_{\alpha=4}^{\infty}\frac{2}{\alpha!}\frac{K^{\alpha/4}}{G^{(\alpha/2)-1}}\{C_{\alpha+2,\alpha/4} + \alpha C_{\alpha-1,(\alpha/4)-1} - 2C_{\alpha,(\alpha/4)-1}\}\hat{q}^\alpha = 0. \tag{5.39}$$

Since q and p are operators, the coefficient of $q^\alpha p^{\alpha-4n}$ must vanish identically for all choices of α and n. This is true if $C_{\alpha,n}$ satisfies

$$C_{\alpha+2,n} - C_{\alpha+1,n} + (\alpha-4n+1)[\alpha C_{\alpha-1,n-1} - (\alpha-4n+2)C_{\alpha,n-1}] = 0, \tag{5.40}$$

for $(\alpha-2)/4 \geq n \geq 1$, $\alpha \geq 2$;

$$C_{\alpha,0} = 1, \quad \text{for} \quad \alpha > 2; \quad C_{\alpha,n} = 0, \quad \text{for} \quad n \geq (\alpha-1)/4. \tag{5.41}$$

$$C_{\alpha,n} = 0, \quad \text{for} \quad \alpha < 2 \quad \text{or} \quad n < 0. \tag{5.42}$$

It can be seen by direct substitution that (5.40) is satisfied if (5.41) is true and if ($n \geq 1$):

$$C_{\alpha,n} = \sum_{s=-1}^{\alpha-2n-3}(\alpha-4n-2-s)[(\alpha-4n-1-s)C_{\alpha-3-s,n-1} - (\alpha-3-s)C_{\alpha-4-s,n-1}]. \tag{5.43}$$

(5.42) is automatically true because of the form we have chosen for $b_{\alpha,p}$, Eq. (5.27).

Directions for writing down the $C_{\alpha,n}$ explicitly are given in the Appendix.

6. THE SCATTERING TIME-DELAY OPERATOR

In recent years there has been an interest in the delay, whether positive or negative, in the motion of a scattered particle due to its interaction with the scattering center.[8–10] Smith[11] showed that the average delay times are given by the eigenvalues of an operator $\hat{Q}$. Lippmann observed that $\hat{Q}$ could be written in the form

$$\hat{Q} = -\hat{S}\hat{T}\hat{S}^*, \tag{6.1}$$

where S is the S matrix and $\hat{T}$ is an operator whose form in the energy representation is

$$\hat{T} = -i\hbar\partial/\partial E. \tag{6.2}$$

Recently Lippmann[12] has given an explicit form for $\hat{T}$ while pointing out that $\hat{T}$ has no eigenfunctions in Hilbert space. Lippmann's $\hat{T}$ is the three-dimensional form of the free-particle time operator written in spherical polar coordinates. The result (6.2) is far more general than this, however, since (6.2) is an appropriate form for $\hat{T}$ in the case of any Hamiltonian with continuous energy eigenvalues.

7. RELATIVISTIC QUANTUM MECHANICS

The real significance of super Hilbert space lies in relativistic quantum mechanics. Since a future paper is planned on this subject, we mention only a few points here.

A 4-operator, which transforms under the Lorentz transformation like a Lorentz 4-vector, is called a "Lorentz 4-operator." Two Lorentz 4-operators $\hat{B}^\mu$ and $\hat{A}_\nu$ which satisfy

$$[\hat{B}^\mu, \hat{A}_\nu] = -i\hbar\delta^\mu_\nu, \tag{7.1}$$

where δ^μ_ν is the Kronecker delta, are called "canonical conjugates." If an operator has a canonical conjugate, we call it a "canonical" operator. A Hermitian canonical Lorentz 4-operator is called a "4-observable." Each of the four components of a 4-observable is called an "observable."

Consider the 4-observable $\hat{q}^\mu \equiv (\hat{x}/c, \hat{y}/c, \hat{z}/c, \hat{T})$, defined by the representation $(f|\,\hat{q}_\nu = (q_\nu f|$, where the Minkowski metric implied has the signature $(1, 1, 1, -1)$. The most general representation of a 4-operator $\hat{p}^\mu$ which satisfies

$$[\hat{p}^\mu, \hat{q}_\nu] = -i\hbar\delta^\mu_\nu \tag{7.2}$$

is

$$(f|\,\hat{p}^\mu \equiv (-i\hbar\partial f/\partial q_\mu + A^\mu f|, \tag{7.3}$$

where $\hat{A}^\mu$ is any 4-observable, defined formally by the representation $(f|\,\hat{A}^\mu \equiv (A^\mu f|$, which commutes with $\hat{q}_\nu$. The representation of $\hat{p}^\mu$ implies that for any $|\psi\rangle$ in $\mathfrak{D}(\hat{p}^\mu)$,

$$\hat{p}^\mu\,|\psi\rangle = (-i\hbar\partial/\partial q_\mu + \hat{A}^\mu)\,|\psi\rangle. \tag{7.4}$$

This is a generalized covariant Schrödinger equation. Thus the Schrödinger equation is just a restatement of the commutation relations and, as such, is not just a nonrelativistic approximation, but is always true. We can write (7.4) in operator form as

$$\hat{p}^\mu = -i\hbar\partial/\partial q_\mu + \hat{A}^\mu. \tag{7.5}$$

In addition to the commutation relations, we must have an invariant equation of motion which specifies the system about which we are talking. The simplest such equation which leads to nontrivial results is

$$\gamma_\mu\hat{p}^\mu + mc\hat{I} = 0, \tag{7.6}$$

where the mc is introduced to make γ_μ dimensionless and γ_μ is a numerical Hermitian Lorentz 4-vector. If we take γ_μ as the Dirac matrices, then (7.5) and (7.6) give the Dirac equation. If we choose the equation

$$\hat{p}^\mu\hat{p}_\mu + m^2c^4\hat{I} = 0, \tag{7.7}$$

we get the Klein–Gordon equation.

If $[\hat{A}^\mu, \partial/\partial q_\nu] \neq 0$ for all μ and ν, or if the invariant equation specifying the specific system involves both $\hat{p}^\mu$ and $\hat{q}^\mu$, the four components of $\hat{p}^\mu$ do not commute. By their definition, however, the four components of $\hat{q}^\mu$ always commute. The nonrelativistic $\hat{T}$ found in Sec. 5 does not commute with $\hat{x}$ because the initial function space is formed of functions of only space variables.

8. NORMS AND THE SPECTRAL THEOREM

It is not possible to introduce a norm in $\mathfrak{W}$ as a whole and it follows that there is no spectral theorem or resolution of the identity in $\mathfrak{W}$ as a whole. It is possible to introduce a norm in certain subspaces of $\mathfrak{W}$, however. For instance, a subspace $\mathfrak{I}$ of $\mathfrak{W}$ can be put into one-to-one correspondence with the space I of all functions whose absolute square is integrable on any bounded region and which are bounded by some polynomial for sufficiently large x through the relation

$$\langle F\,|\,g) \equiv \int_{-\infty}^{\infty} dx e^{-\alpha x} g(x) f^*(x), \tag{8.1}$$

for any $\alpha > 0$, $(g| \in I$, $f \in I$, $\langle F| \in \mathfrak{I}$. We then can define the α norm of $\langle F|$ by

$$\|\langle F|\|_\alpha \equiv \int_{-\infty}^{\infty} dx e^{-\alpha x}\,|f(x)|^2 = \langle F\,|\,f). \tag{8.2}$$

[8] D. Bohm, *Quantum Theory* (Prentice-Hall, Inc., Englewood Cliffs, N.J., 1951), pp. 257–261.
[9] L. Eisenbud, dissertation, Princeton University, 1948.
[10] E. P. Wigner, Phys. Rev. **98**, 145 (1955).
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Note that one can introduce a norm in any self-compatible subspace by letting $\|\langle F|\| = (\langle F|f\rangle)^{\frac{1}{2}}$. A measure space can be constructed on $\mathfrak{W}$ as follows. Let

$$G(A_1, A_2) \equiv \{\langle f|: A_1 < |\langle f|g\rangle| \leq A_2\} \quad (8.3)$$

for all $|g)$ in S, such that $|\langle g|g\rangle| = 1$. Then the set of all $G(A_1, A_2)$ plus the empty set is a semiring. The set of all finite unions of the $G(A_1, A_2)$ is the minimal ring over this semiring. The union of all the semirings is $\mathfrak{W}$. Since $\mathfrak{W}$ belongs to the minimal ring [being $G(0, \infty)$], the minimal ring is a minimal algebra. Since the algebra contains the intersection of any number of its members, it is a Borel algebra and, in fact, it is the minimal Borel algebra over the semiring. Now we can introduce a measure μ on the semiring by

$$\mu(G(A_1, A_2)) = A_2 - A_1. \quad (8.4)$$

One spectral measure in $\mathfrak{W}$ is to let the spectral measure of a set M be its characteristic function.

Since a spectral measure can be found for $\mathfrak{W}$ as a whole, a spectral theorem can be proved in any self-compatible subspace of $\mathfrak{W}$.

Since the whole spectrum of the usual operators used in quantum mechanics appear as eigenvalues with associated eigenkets in super Hilbert space, it is reasonable to speculate that it is the eigenvalues of an operator which represent the expected values of the associated dynamic variable rather than the entire spectrum, as in a Hilbert space.

9. THE UNCERTAINTY PRINCIPLE

Let $\mathfrak{F}$ be a self-compatible subspace of $\mathfrak{W}$ and let $\langle\Phi| \in \mathfrak{F}$. Let $\hat{A}$ and $\hat{B}$ be canonically conjugate Hermitian operators upon $\mathfrak{F}$. Let $\langle\Phi|\Phi) \equiv \|\Phi\|^2$, for all $\langle\Phi|$ in $\mathfrak{F}$. Then, following von Neumann,[13]

$$\begin{aligned} 2\,\mathrm{Im}\,(\Phi|\hat{A}\hat{B}|\Phi\rangle &= -i((\Phi|\hat{A}\hat{B}|\Phi\rangle - \langle\Phi|\hat{B}\hat{A}|\Phi)) \\ &= -i(\Phi|\hat{A}\hat{B} - \hat{B}\hat{A}|\Phi\rangle = \hbar\,\||\Phi\rangle\|^2. \end{aligned} \quad (9.1)$$

Then, by the Schwarz inequality,

$$\begin{aligned} \||\Phi\rangle\|^2 = (2/\hbar)\,\mathrm{Im}\,(\Phi|\hat{A}\hat{B}|\Phi\rangle &\leq (2/\hbar)\,|(\Phi|\hat{A}\hat{B}|\Phi\rangle| \\ &\leq (2/\hbar)\,\|\hat{A}|\Phi\rangle\|\,\|\hat{B}|\Phi\rangle\|. \end{aligned} \quad (9.2)$$

We can rewrite (9.2) as

$$\frac{\|\hat{A}|\Phi\rangle\|\,\|\hat{B}|\Phi\rangle\|}{\||\Phi\rangle\|^2} \geq \frac{\hbar}{2}. \quad (9.3)$$

[13] J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Princeton, N.J., 1955), p. 234.

We define $\bar{A}$, $\bar{B}$, ΔA, and ΔB by

$$\begin{aligned} \bar{A} &\equiv (\Phi|\hat{A}|\Phi\rangle, & \bar{B} &\equiv (\Phi|\hat{B}|\Phi\rangle, \\ \Delta A &\equiv \frac{\|(\hat{A} - \bar{A}\hat{I})|\Phi\rangle\|}{\||\Phi\rangle\|}, & \Delta B &\equiv \frac{\|(\hat{B} - \bar{B}\hat{I})|\Phi\rangle\|}{\||\Phi\rangle\|}. \end{aligned} \quad (9.4)$$

Since $(\hat{A} - \bar{A}\hat{I})$ and $(\hat{B} - \bar{B}\hat{I})$ have the properties assumed above for $\hat{A}$ and $\hat{B}$, respectively, (9.3) holds for them as well and we have

$$(\Delta A)(\Delta B) \geq \hbar/2. \quad (9.5)$$

Now consider a sequence of kets $\{|\Phi_j\rangle\}$ in $\mathfrak{F}$, each satisfying the above, which converge to $|\Phi\rangle$. If the limits exist, we can define ΔA and ΔB by

$$\begin{aligned} \Delta A &\equiv \lim_{j\to\infty} \frac{\|(\hat{A} - \bar{A}_j\hat{I})|\Phi_j\rangle\|}{\||\Phi_j\rangle\|}, \\ \Delta B &\equiv \lim_{j\to\infty} \frac{\|(\hat{B} - \bar{B}_j\hat{I})|\Phi_j\rangle\|}{\||\Phi_j\rangle\|}. \end{aligned} \quad (9.6)$$

Since (9.5) is true for all j,

$$\Delta A\Delta B = \lim_{j\to\infty} \Delta A_j \lim_{k\to\infty} \Delta B_k = \lim_{j\to\infty} \Delta A_j \Delta B_j \geq \hbar/2. \quad (9.7)$$

We call ΔA and ΔB the uncertainty in state $|\Phi\rangle$ of $\hat{A}$ and $\hat{B}$, respectively.

Thus every pair of Hermitian canonically conjugate operators $\hat{A}$ and $\hat{B}$ upon a self-compatible subspace of $\mathfrak{W}$ obeys an uncertainty principle with regard to kets in that space and kets which are limits of sequences of kets in that space, such that ΔA and ΔB exist.

10. CONCLUSION

In addition to combining free- and bound-state problems into a natural whole and allowing the existence of a time operator which will be useful in its own right, super Hilbert space allows relativistic quantum mechanics to be based on a simple, natural, four-dimensional commutation relation. It may be that this basis and the representation of states by functionals rather than functions will contribute to the solution of some of the problems of relativistic quantum mechanics.

ACKNOWLEDGMENTS

My deepest thanks to Dr. Duane Montgomery of the Institute for Defense Analyses (IDA), without whose endless patience and forebearance in helping me to learn the elements of analysis and wise advice on numerous problems, this paper could not have been done. I also owe a debt of gratitude to Dr. Robert Kupperman of IDA and Professor Harvey Smith of

Oakland University (Michigan), who read a first draft and answered a number of important mathematical questions for me.

APPENDIX: DIRECTIONS FOR WRITING DOWN $C_{\alpha,n}$

$C_{\alpha,n}$ can now be written in terms of the symbols R and F, which do not commute, as

$$C_{\alpha,n} = -2[R(R+F)^{n-1}]_{\alpha,n}, \quad \text{for} \quad n > 0,$$
$$= 1, \quad \text{for} \quad n = 0, \quad \text{(A1)}$$

where the subscripts α, n refer to the values to be used in the rules below. Thus for $n > 0$, $C_{\alpha,n}$ has $2^{(n-1)}$ terms, each of which has 2^n symbols. Consider a term with N_R R's and N_F F's. We define A_i as follows:

$$A_i \equiv 0, \text{ for } i = 0,$$
$$\equiv A_{i-1} + 1, \text{ for an } R \text{ symbol},$$
$$\equiv A_{i-1} + 2, \text{ for an } F \text{ symbol}. \quad \text{(A2)}$$

Going from left to right in order, for the first R symbol we write

$$\sum_{j_1=-1}^{\alpha-2n-3} (\alpha - 4n - 2 - j_1) \quad \text{(A3)}$$

and for each succeeding R symbol

$$-2[2(n-t)+3] \sum_{j_r=j_{r-1}}^{\alpha-2n-2-r} (\alpha - 4n - 2 + A_t - j_r), \quad \text{(A4)}$$

where the index r refers to 1 plus the number of R's to the left of the R under consideration and the index t refers to 1 plus the number of factors (R or F) to the left of the R under consideration. For example, consider

$$r = 1 \quad 23 \quad 4$$
$$RFRRFR$$
$$t = 1\,2\,3\,4\,5\,6.$$

For each F we write

$$(\alpha - 4n - 2 - j_i + A_t)(\alpha - 4n - 3 - j_i + A_t), \quad \text{(A5)}$$

where i has the same value as that of the r in the first R to the left and t refers to the position of F, as above.

We now show that these directions specify a $C_{\alpha,n}$ which satisfies (5.41) and (5.43). Consider $C_{\alpha-3-s,n-1}$. The directions are to write

$$\sum_{j_1'=-1}^{\alpha-2n-4-s} [\alpha - 4n - 1 - (j_1' + s)] \quad \text{(A6)}$$

for the first R,

$$-2[2(n-1-t)+3] \times \sum_{j_r'=j_{r-1}'}^{\alpha-2n-3-r-s} [\alpha - 4n - 1 + A_t - (j_r' + s)] \quad \text{(A7)}$$

for succeeding R's, and

$$(\alpha - 4n - 1 + A_t - (j_i' + s)) \times (\alpha - 4n - 2 + A_t - (j_i + s)) \quad \text{(A8)}$$

for each F. If we define $j_r \equiv j_r' + s + 1$, the directions become

$$\sum_{j_1=s-1}^{\alpha-2n-4} (\alpha - 4n - j_1 - 1) \quad \text{(A9)}$$

for the first R,

$$-2[2(n-(t+1))+3] \times \sum_{j_r=j_{r-1}}^{\alpha-2n-3-r} (\alpha - 4n - 1 + A_t - j_r) \quad \text{(A10)}$$

for succeeding R's, and

$$(\alpha - 4n - 1 + A_t - j_i)(\alpha - 4n - 2 + A_t - j_i) \quad \text{(A11)}$$

for each F. We can get the directions for $C_{\alpha-4-s,n-1}$ by letting $\alpha \to \alpha - 1$ in the directions for $C_{\alpha-3-s,n-1}$. If at the same time we let $j_r \to j_r - 1$, we get as the directions for $C_{\alpha-4-s,n-1}$

$$\sum_{j_1=s}^{\alpha-2n-4} (\alpha - 4n - j_1 - 1) \quad \text{(A12)}$$

for the first R,

$$-2[2(n-(t+1))+3] \times \sum_{j_r=j_{r-1}}^{\alpha-2n-2-(r+1)} (\alpha - 4n - 1 + A_t - j_r) \quad \text{(A13)}$$

for succeeding R's, and

$$(\alpha - 4n - 1 + A_t - j_i)(\alpha - 4n - 2 + A_t - j_i) \quad \text{(A14)}$$

for each F. Thus the only difference between $C_{\alpha-3-s,n-1}$ and $C_{\alpha-4-s,n-1}$ is that the lower bound on the summation for the first R is $(s-1)$ for $C_{\alpha-3-s,n-1}$ and (s) for $C_{\alpha-4-s,n-1}$. Thus

$$(\alpha - 4n - 1 - s)C_{\alpha-3-s,n-1} - (\alpha - 3 - s)C_{\alpha-4-s,n-1}$$
$$= (-4n+2)C_{\alpha-4-s,n-1} + (\alpha - 4n - 1 - s)(\alpha - 4n - s)D_{\alpha-3-s,n-1}, \quad \text{(A15)}$$

where $D_{\alpha-3-s,n-1}$ has $n-2$ factors and is the same as $C_{\alpha-3-s,n-2}$, except that the first summation is dropped

and the lower limit on the second summation is $j_2 = s - 1$. Thus

$$C_{\alpha,n} = \sum_{s=-1}^{\alpha-2n-3} (\alpha - 4n - 2 - s)(-4n + 2)C_{\alpha-4-s,n-1} + \sum_{s=-1}^{\alpha-2n-3} (\alpha - 4n - s)(\alpha - 4n - 1 - s) \times (\alpha - 4n - 2 - s)D_{\alpha-3-s,n-1}. \quad \text{(A16)}$$

Consider the first term. Let us rename the indices r, t, and j_r in the rules for $C_{\alpha-4-s,n-1}$, so that $t' \equiv t + 1$, $r' \equiv r + 1$, and $(j_r')' = j_{r-1}'$, and at the same time let $s \equiv j_1$. Then the first two factors in the first term in (A16) become

$$\left[\sum_{j_1=-1}^{\alpha-2n-3} (\alpha - 4n - 2 - j_1)\right] \times \left[(-4n + 2) \sum_{j_2=j_1}^{\alpha-2n-4} (\alpha - 4n - 1 - j_1)\right], \quad \text{(A17)}$$

which is just R^2, and the directions for the rest of the terms are just (we have dropped the primes on r, t, and j_r):

$$-2[2(n - t) + 3] \times \sum_{j_r=j_{r-1}}^{\alpha-2n-2-4} (\alpha - 4n - 1 + A_{(t-1)} - j_r) \quad \text{(A18)}$$

for each succeeding R ($r > 2$) and

$$(\alpha - 4n - 1 - j_i + A_{(t-1)}) \times (\alpha - 4n - 2 - j_i + A_{(t-1)}) \quad \text{(A19)}$$

for each succeeding F ($t > 2$). Since the order of the factors after R^2 is the same as the order of the factors in $C_{\alpha-4-s,n-1}$ after R [the only difference being that what was the jth factor in $C_{\alpha-4-s,n-1}$ is the $(j + 1)$th factor in the first term on the right-hand side of (A16)] it follows that if we want the directions for determining A_i to apply to the first term on the right-hand side of (A16), where the index refers to the position of a factor in that term, we must let $A_{t-1} \to (A_t - 1)$ in (A18) and (A19). Having made this change in (A18) and (A19), we see that the rules for the first term on the right-hand side of (A16) are the same as those for $R^2(R + F)_{\alpha,n}^{n-2}$. Similarly, one can show that the second term on the right-hand side of (A16) is $RF(R + F)_{\alpha,n}^{n-2}$. Thus

$$\begin{aligned} C_{\alpha,n} &= R^2(R + F)_{\alpha,n}^{n-2} + RF(R + F)_{\alpha,n}^{n-2} \\ &= R(R + F)(R + F)_{\alpha,n}^{n-2} = R(R + F)_{\alpha,n}^{n-1} \\ &= \sum_{s=-1}^{\alpha-2n-3} (\alpha - 4n - 2 - s)[(\alpha - 4n - 1 - s) \times C_{\alpha-3-s,n-1} - (\alpha - 3 - s)C_{\alpha-4-s,n-1}]. \end{aligned} \quad \text{(A20)}$$

Exact Robertson–Walker Cosmological Solutions Containing Relativistic Fluids*

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(Received 21 September 1968)

A new derivation of the Robertson–Walker metrics is presented which elucidates the relationship between these spatially homogeneous and isotropic models and certain spatially homogeneous but anisotropic models ("three-cylinder universes"). The evolutionary equations for Robertson–Walker models containing as many as four distinct noninteracting relativistic fluids (each obeying a gamma-law equation of state) are examined, and 25 exact closed-form solutions of this type are presented explicitly.

INTRODUCTION

Recently, several writers have discussed cosmological models of the Robertson–Walker type containing both radiation and incoherent dust (pressureless matter).[1–5] Under the assumption that the radiation and the matter do not interact, exact solutions may be derived[3–7] which evolve, during early epochs, very much like exact solutions containing only radiation,[8,5] and during late epochs, like the exact solutions of Friedmann[9] which contain only incoherent dust.

In early stages of the expansion of the fireball when temperatures are in the range of 10^{12}–10^{13}°K or higher, because of the strong interactions of the mesons (π, K, etc.) which appear at these temperatures, the equation of state of the matter (assuming thermodynamic equilibrium) is not well known, but in any case, the pressure due to matter is not negligible. Accordingly, even if one ignores the actual interactions which do in fact occur between the radiation and the matter, it seems desirable to obtain still more exact solutions of the Robertson–Walker type corresponding to various equations of state for the matter. Eighteen exact solutions which have not (to my knowledge) previously appeared in the literature are presented here, and for the sake of completeness, seven previously published solutions are also given, using the same notation throughout.

As an alternative to the homogeneous and isotropic Robertson–Walker cosmological models, there has been some interest recently in homogeneous but anisotropic models which are spatially closed in two directions but open in the third direction (three-cylinder cosmologies). Such models have been derived by Thorne,[10] Kantowski and Sachs,[11] and Doroshkevich.[12] A new derivation of the Robertson–Walker metrics is presented here which elucidates the relationship between the Robertson–Walker models and the three-cylinder models.

Derivation of the Robertson–Walker Metrics

We assume that the space–time manifold is spherically symmetric and endowed with a sufficiently differentiable metric tensor field. We further assume that the matter in the space–time moves on a differentiable congruence of geodesic world-lines. It is then possible[5] to construct orthogonal comoving coordinates $(\tau, \chi, \theta, \phi)$ on coordinate patches on the space–time. In terms of these coordinates, the metric has the form[5]

$$ds^2 = d\tau^2 - f^2(\tau, \chi)\, d\chi^2 - S^2(\tau, \chi)\, d\Omega^2, \quad \text{(1a)}$$

$$d\Omega^2 = d\theta^2 + \sin^2\theta\, d\phi^2, \quad \text{(1b)}$$

where f and S are differentiable scalar fields defined on each coordinate patch.

The scalar field S may be interpreted as the intrinsic radius of curvature of the two-sphere defined by the locus of points $\tau =$ constant, $\chi =$ constant. It is important to note that $\delta_\mu S$ (the four-gradient of S) need not, *a priori*, be a spacelike vector: it may be spacelike, null, or timelike, or it may vanish. Only if $\delta_\mu S$ is spacelike is it possible to write the metric in the usual form

$$ds^2 = A^2(t, r)\, dt^2 - B^2(t, r)\, dr^2 - r^2\, d\Omega^2,$$
$$A^2 > 0, \quad B^2 > 0.$$

(For a complete discussion of the role of $\delta_\mu S$ in the

* Work performed under the auspices of the U.S. Atomic Energy Commission.

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theory of spherically symmetric space-times, see Ref. 5.)

The components of the Einstein tensor when referred to the orthonormal tetrad of one-forms

$$\omega^0 = d\tau, \qquad \omega^2 = S(\tau, \chi)\, d\theta,$$
$$\omega^1 = f(\tau, \chi)\, d\chi, \quad \omega^3 = S(\tau, \chi) \sin\theta\, d\phi, \tag{2}$$

may then be found very efficiently by Misner's prescription for computing curvature.[13] The Einstein field equations without cosmological constant are then

$$G_{00} = \frac{\dot{S}}{S}\left(\frac{\dot{S}}{S} + 2\frac{\dot{f}}{f}\right) - \frac{1}{f^2}\left[2\frac{S''}{S} + \frac{S'}{S}\left(\frac{S'}{S} - 2\frac{f'}{f}\right)\right] + \frac{1}{S^2} = \kappa\mu, \tag{3}$$

$$G_{01} = \frac{\dot{S}'}{S} - \frac{\dot{f}}{f}\frac{S'}{S} = 0, \tag{4}$$

$$G_{11} = \frac{1}{f^2}\left(\frac{S'}{S}\right)^2 - 2\frac{\ddot{S}}{S} - \left(\frac{\dot{S}}{S}\right)^2 - \frac{1}{S^2} = \kappa p_r, \tag{5}$$

$$G_{22} = \frac{1}{f^2}\left(\frac{S''}{S} - \frac{f'}{f}\frac{S'}{S}\right) - \frac{\ddot{f}}{f} - \frac{\ddot{S}}{S} - \frac{\dot{f}}{f}\frac{\dot{S}}{S} = \kappa p_a, \tag{6}$$

where μ is the proper mass–energy density of matter, p_r is the component of stress in the radial direction (that is, in the χ direction), p_a is the component of stress in the angular directions (that is, in any direction tangent to a two-sphere τ = constant, χ = constant), and $\kappa = 8\pi G/c^4$ is the relativistic gravitational constant. Differentiation with respect to τ is denoted by a dot; with respect to χ, by a prime. The conservation laws

$$T^{\mu\nu}{}_{;\nu} = 0$$

will also be useful in the discussion below; these are

$$\dot{\mu} + \mu\left(\frac{\dot{f}}{f} + 2\frac{\dot{S}}{S}\right) + p_r\frac{\dot{f}}{f} + 2p_a\frac{\dot{S}}{S} = 0, \tag{7}$$

$$p_r' + 2\frac{S'}{S}(p_r - p_a) = 0. \tag{8}$$

If we now assume that the distribution of matter on each spacelike hypersurface τ = constant is homogeneous, that is,

$$\mu = \mu(\tau), \quad p_r = p_r(\tau), \quad p_a = p_a(\tau), \tag{9}$$

then p_r' vanishes identically. The conservation law (8) may then be satisfied by any of the following choices:

(A) $S' \neq 0$ and $p_r = p_a = p(\tau)$, (10)

(B) $S' = 0$ and $p_r \neq p_a$, (11)

(C) $S' = 0$ and $p_r = p_a = p(\tau)$. (12)

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The choices (B) and (C) lead to space-times whose spacelike hypersurfaces τ = constant are three-cylinders, i.e., to spherically symmetric space-times which are spatially homogeneous but anisotropic. Such space-times have been discovered by Thorne,[10] Kantowski and Sachs,[11] and Doroshkevich.[12]

Our present interest, however, is only the choice (A). Substituting (10) into the conservation law (7), we see that the expression $[(\dot{f}/f) + 2(\dot{S}/S)]$ must be independent of χ. Thus we conclude that

$$f(\tau, \chi)S^2(\tau, \chi) = g(\tau)h(\chi), \tag{13}$$

where g and h are as yet undetermined functions. Now the field equation (4) may be integrated once to give

$$S'(\tau, \chi) = m(\chi)f(\tau, \chi), \tag{14}$$

where m is an undetermined function.

What forms must f and S have in order to satisfy both (13) and (14)? Solving (13) for S, differentiating once with respect to χ, and using (14), we obtain the relation

$$\frac{d}{d\chi}[h(\chi)]^{\frac{1}{2}} = [h(\chi)]^{\frac{1}{2}}\frac{f'(\tau, \chi)}{f(\tau, \chi)} + m(\chi)\left[\frac{f^3(\tau, \chi)}{g(\tau, \chi)}\right]^{\frac{1}{2}}. \tag{15}$$

For each value of χ, this relation must hold identically for all values of τ. This is possible only if f'/f and f^3/g are both independent of τ, that is, if f can be decomposed into a product of a function of τ with a function of χ:

$$f(\tau, \chi) = A(\tau)B(\chi), \quad \text{where} \quad A^3(\tau) = g(\tau). \tag{16}$$

We then find from (14) that S is also decomposable:

$$S(\tau, \chi) = A(\tau)M(\chi). \tag{17}$$

It is apparent from (16) and the form of the metric (1) that there is no loss of generality in setting $B(\chi) = 1$; this corresponds merely to a suitable choice of the coordinate χ. Thus the metric becomes

$$ds^2 = d\tau^2 - A^2(\tau)[d\chi^2 + M^2(\chi)\, d\Omega^2]. \tag{18}$$

We now find that the field equations (3), (5), and (6) can be written in the form

$$2\frac{M''}{M} + \left(\frac{M'}{M}\right)^2 - \frac{1}{M^2} = K' = 3\dot{A}^2 - \kappa A^2\mu, \tag{19}$$

$$\left(\frac{M'}{M}\right)^2 - \frac{1}{M^2} = K = \dot{A}^2 + 2A\ddot{A} + \kappa A^2 p, \tag{20}$$

$$\frac{M''}{M} = K = \dot{A}^2 + 2A\ddot{A} + \kappa A^2 p, \tag{21}$$

where we have introduced separation constants K and

K', since the left-hand member of each equation is a function only of χ and the right-hand member, a function only of τ. We find at once that

$$K' = 3K. \tag{22}$$

We may now integrate the left-hand member of (21). Depending on the value of K, we obtain three different results:

$$\begin{aligned} M(\chi) &= D \sin [(|K|)^{\frac{1}{2}}\chi + \alpha], && K < 0, \\ &= D'(\chi + \beta), && K = 0, \\ &= E \exp [-(K)^{\frac{1}{2}}\chi] + E' \exp [(K)^{\frac{1}{2}}\chi], && K > 0, \end{aligned} \tag{23}$$

where D, D', α, β, E, and E' are constants of integration.

Substituting these expressions into the remaining field equations (19) and (20), we find

$$\begin{aligned} D &= (|K|)^{-\frac{1}{2}}, && K < 0, \\ D' &= 1, && K = 0, \\ EE' &= -1/(4K), && K > 0. \end{aligned} \tag{24}$$

Since α, β, and E/E' merely fix the origin of the coordinate χ and thus have no intrinsic geometrical significance, we pick

$$\begin{aligned} \alpha &= \beta = 0, \\ E &= -E'. \end{aligned} \tag{25}$$

We next note that multiplying K by any positive number λ has the effect of changing the scale of χ by a factor of $(\lambda)^{\frac{1}{2}}$. Thus there is no loss of generality in considering only $K = -1$, 0, or $+1$. We thus obtain the three Robertson–Walker metrics

$$ds^2 = d\tau^2 - A^2(\tau)[d\chi^2 + \sin^2 \chi \, d\Omega^2], \qquad K = -1, \tag{26a}$$

$$ds^2 = d\tau^2 - A^2(\tau)[d\chi^2 + \chi^2 \, d\Omega^2], \qquad K = 0, \tag{26b}$$

$$ds^2 = d\tau^2 - A^2(\tau)[d\chi^2 + \sinh^2 \chi \, d\Omega^2], \qquad K = +1. \tag{26c}$$

These describe space–times which are spatially homogeneous and isotropic. The spacelike hypersurfaces $\tau =$ constant are spaces of constant curvature, respectively positive, zero, and negative. The space–times described by the above forms will be referred to in the rest of the discussion as *closed*, *flat*, and *hyperbolic* Robertson–Walker space–times, respectively.

The function $A(\tau)$, which describes the evolution of the geometry, and the functions $\mu(\tau)$ and $p(\tau)$, which describe the behavior of the matter in these space–times, remain to be found. These functions appear in the three Eqs. (7), (19), and (20); because of the Bianchi identities, however, only two of these equations are independent. Thus, in order to obtain unique solutions, it is necessary to provide additional information about these functions. This information may be given most conveniently in the form of an equation of state of the matter in the space–time, that is, in the form of a functional relation between μ and p. [Alternatively, of course, one can simply specify an *ad hoc* explicit form for $A(\tau)$ and calculate μ and p from the field equations (19) and (20), as McIntosh has done.[1] There is no guarantee, however, that this procedure will result in a physically reasonable form of matter.]

With the aid of (10) and (17), the conservation law (7) may now be written as

$$\dot{\mu} + 3(\mu + p)\dot{A}/A = 0. \tag{27}$$

Given the equation of state relating p and μ, this equation may be integrated (at least in principle) to give μ as a function of A. The field equation (19) may then be solved to obtain A as an implicit function of τ:

$$\int \frac{dA}{[K + \frac{1}{3}\kappa A^2 \mu(A)]^{\frac{1}{2}}} = \tau - \tau_0, \tag{28}$$

where τ_0 is a constant of integration.

Conformal Coordinates

As we shall see in the discussion below, there are several cases of interest in which the solution (28) is an elliptic function. In some of these cases, a coordinate transformation which we now describe permits us to reduce the relevant quadratures to elementary functions.

If we define a new timelike coordinate by

$$d\psi = d\tau/A(\tau) \tag{29}$$

and then express A as a function of ψ instead of τ, we can write the metrics (26) in the forms

$$ds^2 = A^2(\psi)[d\psi^2 - d\chi^2 - \sin^2 \chi \, d\Omega^2], \qquad K = -1, \tag{30a}$$

$$ds^2 = A^2(\psi)[d\psi^2 - d\chi^2 - \chi^2 \, d\Omega^2], \qquad K = 0, \tag{30b}$$

$$ds^2 = A^2(\psi)[d\psi^2 - d\chi^2 - \sinh^2 \chi \, d\Omega^2], \qquad K = +1. \tag{30c}$$

Since the metric forms on any two neighborhoods of a (ψ, χ) coordinate plane in such a spacetime are conformally related, we call the coordinates ψ and χ *conformal coordinates*.

We now find that $A(\tau)$ may be given in parametric form, with ψ as parameter. The expression (28) is then replaced by

$$\int \frac{dA}{A[K + \frac{1}{3}\kappa A^2\mu(A)]^{\frac{1}{2}}} = \psi, \tag{31a}$$

$$\tau - \tau_0 = \int A(\psi)\, d\psi. \tag{31b}$$

The expression (31b), of course, is essentially identical to (28); in some cases, however, (31a) may be expressed in terms of elementary functions, while (31b) is an elliptic function. In such cases, an exact, closed-form solution may be given for the metric (30).

Relativistic Fluids

We now consider the equation of state

$$p = (\gamma - 1)\mu, \quad \mu + p = \gamma\mu, \quad 1 \leq \gamma \leq 2, \tag{32}$$

where γ is a constant. (The limits on γ result from the requirements that the stresses be pressures rather than tensions and that the speed of sound in the fluid be less than the speed of light *in vacuo*.) For $\gamma = 1$, the pressure vanishes, so that the equation of state is that of incoherent dust. For $\gamma = \frac{4}{3}$, the equation of state is that of a photon gas or a gas of noninteracting relativistic particles.

For this equation of state, the conservation law (27) may be integrated to give

$$\mu(\tau) = B/A^{3\gamma}(\tau), \tag{33}$$

where B is a constant of integration. We now see that, for $K \neq 0$, (28) may be readily expressed in terms of elementary functions or elliptic integrals only if $(3\gamma - 2)$ is an integer (see, e.g., §2.29 of Ref. 14), that is, if

$$\gamma = n/3, \quad n = 3, 4, 5, 6, \tag{34}$$

while (31a) may be expressed in closed form for arbitrary K and arbitrary γ.[15] Exact closed-form solutions for these cases are presented explicitly in Appendix A.

Consider now a fluid composed of two or more components, each characterized by a different value of γ. If the various components are strictly noninteracting, then the conservation law applies to each component *separately*, and each component then satisfies (33). The total proper mass–energy density of the fluid is then

$$\mu = \frac{B_1}{A^{3\gamma_1}(\tau)} + \frac{B_2}{A^{3\gamma_2}(\tau)} + \cdots, \tag{35}$$

where γ_i characterizes the equation of state of the ith component of the fluid, and the total pressure is

$$p = \frac{(\gamma_1 - 1)B_1}{A^{3\gamma_1}(\tau)} + \frac{(\gamma_2 - 1)B_2}{A^{3\gamma_2}(\tau)} + \cdots. \tag{36}$$

The solutions (28) or (31a) may be readily expressed in terms of elementary functions or elliptic functions if there are no more than four components and if each of the γ_i satisfies the condition (34). Closed-form exact solutions for two- and three-component cases are presented in Appendices B and C, respectively. Four-component cases for which the γ_i satisfy (34) can be expressed only in terms of elliptic functions for general values of the integration constants B_i.

APPENDIX A: SINGLE-COMPONENT RELATIVISTIC FLUID CASES

Exact closed-form solutions for Robertson–Walker cosmological models containing a single-component relativistic fluid with equation of state

$$p = (\gamma - 1)\mu$$

are presented below. For convenience, we have given solutions for $\gamma = 1$ (dust), $\gamma = \frac{4}{3}$ (radiation), $\gamma = \frac{5}{3}$, and $\gamma = 2$ in addition to the solutions for arbitrary γ. A key to the solutions is given in Table I.

The behavior of the fluid (not given explicitly below) is in all cases related to the metric function $A(\tau)$ or $A(\psi)$ by

$$\mu = B/A^{3\gamma}, \quad p = (\gamma - 1)B/A^{3\gamma},$$

and the abbreviation

$$a \equiv \kappa B/6$$

is used throughout.

TABLE I. Summary of solutions.

	$\gamma = 1$ $p = 0$	$\gamma = \frac{4}{3}$ $p = \mu/3$	$\gamma = \frac{5}{3}$ $p = 2\mu/3$	$\gamma = 2$ $p = \mu$	Arbitrary γ $p = (\gamma - 1)\mu$
$K = -1$	(A1)[a]	(A4)[b]	(A7)[c]	(A10)[d]	(A13)[e]
$K = 0$	(A2)[a]	(A5)[c]	(A8)[c]	(A11)[c]	(A14)[c]
$K = +1$	(A3)[a]	(A6)[c]	(A9)[c]	(A12)[c]	(A15)[e]

[a] Friedmann (see Ref. 9).
[b] Tolman (see Ref. 8).
[c] Vajk (see Ref. 5).
[d] U. Gerlach, unpublished work, 1965.
[e] Hughston (see Ref. 15).

[14] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series, and Products* (Academic Press Inc., New York, 1965).

[15] The author is grateful to Lane P. Hughston for pointing out that the solutions (A13) and (A15) can be expressed in closed form (private communication, 1968).

Solutions

$\gamma = 1, K = -1$:

$$2a \sin^{-1}[A(\tau)/2a]^{\frac{1}{2}} - [2aA(\tau) - A^2(\tau)]^{\frac{1}{2}} = \tau - \tau_0. \tag{A1a}$$

$$A(\psi) = a(1 - \cos\psi) = 2a \sin^2 \frac{\psi}{2},$$

$$\tau - \tau_0 = a(\psi - \sin\psi) = 2a\left(\frac{\psi}{2} - \sin\frac{\psi}{2}\cos\frac{\psi}{2}\right). \tag{A1b}$$

$\gamma = 1, K = 0$:

$$A(\tau) = \left(\frac{9a}{2}\right)^{\frac{1}{3}}(\tau - \tau_0)^{\frac{2}{3}}. \tag{A2a}$$

$$A(\psi) = \frac{a}{2}\psi^2,$$

$$\tau - \tau_0 = \frac{a}{6}\psi^3. \tag{A2b}$$

$\gamma = 1, K = +1$:

$$[A^2(\tau) + 2aA(\tau)]^{\frac{1}{2}} - 2a \sinh^{-1}[A(\tau)/2a]^{\frac{1}{2}} = \tau - \tau_0. \tag{A3a}$$

$$A(\psi) = a(\cosh\psi - 1) = 2a \sinh^2 \frac{\psi}{2},$$

$$\tau - \tau_0 = a(\sinh\psi - \psi) = 2a\left(\sinh\frac{\psi}{2}\cosh\frac{\psi}{2} - \frac{\psi}{2}\right). \tag{A3b}$$

$\gamma = \frac{4}{3}, K = -1$:

$$A(\tau) = [2a - (\tau - \tau_0)^2]^{\frac{1}{2}}. \tag{A4a}$$

$$A(\psi) = (2a)^{\frac{1}{2}} \sin\psi,$$

$$\tau - \tau_0 = (2a)^{\frac{1}{2}} \cos\psi. \tag{A4b}$$

$\gamma = \frac{4}{3}, K = 0$:

$$A(\tau) = (8a)^{\frac{1}{4}}(\tau - \tau_0)^{\frac{1}{2}}. \tag{A5a}$$

$$A(\psi) = (2a)^{\frac{1}{2}}\psi,$$

$$\tau - \tau_0 = (a/2)^{\frac{1}{2}}\psi^2. \tag{A5b}$$

$\gamma = \frac{4}{3}, K = +1$:

$$A(\tau) = [(\tau - \tau_0)^2 - 2a]^{\frac{1}{2}}. \tag{A6a}$$

$$A(\psi) = (2a)^{\frac{1}{2}} \sinh\psi,$$

$$\tau - \tau_0 = (2a)^{\frac{1}{2}} \cosh\psi. \tag{A6b}$$

$\gamma = \frac{5}{3}, K = -1$:

$$A(\psi) = (2a)^{\frac{1}{3}}[\sin\tfrac{3}{2}\psi]^{\frac{2}{3}},$$

$$\tau - \tau_0 = \int A(\psi)\, d\psi. \tag{A7}$$

$\gamma = \frac{5}{3}, K = 0$:

$$A(\tau) = \left(\frac{25a}{2}\right)^{\frac{1}{5}}(\tau - \tau_0)^{\frac{2}{5}}. \tag{A8a}$$

$$A(\psi) = \left(\frac{9a}{2}\right)^{\frac{1}{3}}\psi^{\frac{2}{3}},$$

$$\tau - \tau_0 = \frac{3}{5}\left(\frac{9a}{2}\right)^{\frac{1}{3}}\psi^{\frac{5}{3}}. \tag{A8b}$$

$\gamma = \frac{5}{3}, K = +1$:

$$A(\psi) = (2a)^{\frac{1}{3}}[\sinh\tfrac{3}{2}\psi]^{\frac{2}{3}},$$

$$\tau - \tau_0 = \int A(\psi)\, d\psi. \tag{A9}$$

$\gamma = 2, K = -1$:

$$A(\psi) = (2a)^{\frac{1}{4}}(\sin 2\psi)^{\frac{1}{2}},$$

$$\tau - \tau_0 = \int A(\psi)\, d\psi. \tag{A10}$$

$\gamma = 2, K = 0$:

$$A(\tau) = (18a)^{\frac{1}{6}}(\tau - \tau_0)^{\frac{1}{3}}. \tag{A11a}$$

$$A(\psi) = (8a)^{\frac{1}{4}}\psi^{\frac{1}{2}},$$

$$\tau - \tau_0 = \tfrac{2}{3}(8a)^{\frac{1}{4}}\psi^{\frac{3}{2}}. \tag{A11b}$$

$\gamma = 2, K = +1$,

$$A(\psi) = (2a)^{\frac{1}{4}}(\sinh 2\psi)^{\frac{1}{2}},$$

$$\tau - \tau_0 = \int A(\psi)\, d\psi. \tag{A12}$$

Arbitrary $\gamma, K = -1$:

$$A(\psi) = (2a)^{1/(3\gamma-2)}\left[\sin\left(\frac{3\gamma - 2}{2}\right)\psi\right]^{2/(3\gamma-2)},$$

$$\tau - \tau_0 = \int A(\psi)\, d\psi. \tag{A13}$$

Arbitrary $\gamma, K = 0$:

$$A(\tau) = (\tfrac{9}{2}\gamma^2 a)^{1/(3\gamma)}(\tau - \tau_0)^{2/(3\gamma)}. \tag{A14a}$$

$$A(\psi) = [(3\gamma - 2)^2 a/2]^{1/(3\gamma-2)}\psi^{2/(3\gamma-2)},$$

$$\tau - \tau_0 = \frac{1}{3\gamma}[(3\gamma - 2)^2 a/2]^{1/(3\gamma-2)}\psi^{3\gamma/(3\gamma-2)}. \tag{A14b}$$

Arbitrary $\gamma, K = +1$:

$$A(\psi) = (2a)^{1/(3\gamma-2)}\left[\sinh\left(\frac{3\gamma - 2}{2}\right)\psi\right]^{2/(3\gamma-2)},$$

$$\tau - \tau_0 = \int A(\psi)\, d\psi. \tag{A15}$$

APPENDIX B: TWO-COMPONENT RELATIVISTIC FLUID CASES

Nine exact closed-form solutions for Robertson–Walker space-times containing two noninteracting relativistic fluids with equations of state

$$p_1 = (\gamma_1 - 1)\mu_1, \quad p_2 = (\gamma_2 - 1)\mu_2$$

are given below for $\gamma_1 = 1, \frac{4}{3}$, or $\frac{5}{3}$, and $\gamma_2 = \frac{4}{3}, \frac{5}{3}$, or 2, with $\gamma_1 < \gamma_2$. In another nine such cases, neither (28) nor (31a) can be readily reduced to closed form: both expressions give elliptic functions. A summary of these two-component fluid cases is presented in Table II.

TABLE II. Summary of solutions.

	$\gamma_2 = \frac{4}{3}$ $p_2 = \mu_2/3$	$\gamma_2 = \frac{5}{3}$ $p_2 = 2\mu_2/3$	$\gamma_2 = 2$ $p_2 = \mu_2$	K
$\gamma_1 = 1$	(B1)[a–d]	Elliptic	Elliptic	−1
$p_1 = 0$	(B2)[c–e]	Elliptic	(B4)	0
	(B3)[c,d]	Elliptic	Elliptic	+1
$\gamma_1 = \frac{4}{3}$		Elliptic	(B6)	−1
$p_1 = \mu_1/3$		(B5)	(B7)	0
		Elliptic	(B8)	+1
$\gamma_1 = \frac{5}{3}$			Elliptic	−1
$p_1 = 2\mu_1/3$			(B9)	0
			Elliptic	+1

[a] G. Lemaître, Am. Soc. Sci. Bruxelles 47A, 49 (1927).
[b] Alpher and Hermann (see Ref. 7).
[c] Chernin (see Ref. 6).
[d] Cohen (see Ref. 4).
[e] Jacobs (see Ref. 3).

The total mass–energy density and total pressure in these solutions are given by

$$\mu = (B_1/A^{3\gamma_1}) + (B_2/A^{3\gamma_2}),$$
$$p = (\gamma_1 - 1)(B_1/A^{3\gamma_1}) + (\gamma_2 - 1)(B_2/A^{3\gamma_2}),$$

respectively, with $\gamma_1 < \gamma_2$. The abbreviations

$$a \equiv \kappa B_1/6, \quad b \equiv B_2/B_1,$$

are used below. Note that, for $b = 0$ (i.e., for $B_2 = 0$), these solutions reduce to the corresponding single-component solution in which $\gamma = \gamma_1$.

Chernin (see Ref. 6) has remarked that the parametrized solutions (B1b), (B2b), and (B3b) for universes containing both dust and radiation may be written, respectively, as sums of the parametrized solutions (A1b), (A2b), and (A3b) for universes containing only dust and the parametrized solutions (A4b), (A5b), and (A6b), respectively, for universes containing only radiation. Hughston[16] has obtained a number of solutions (not given below) for two-component fluids by generalizing this "superposition" property.

[16] L. P. Hughston (submitted to Astrophys. J.).

Solutions

$\gamma_1 = 1, \gamma_2 = \frac{4}{3}, K = -1$:

$$a \sin^{-1} \frac{A(\tau) - a}{[a(a + 2b)]^{\frac{1}{2}}} - [2ab + 2aA(\tau) - A^2(\tau)]^{\frac{1}{2}} = \tau - \tau_0. \quad \text{(B1a)}$$

$$A(\psi) = a + [a(a + 2b)]^{\frac{1}{2}} \sin \psi,$$
$$\tau - \tau_0 = a\psi - [a(a + 2b)]^{\frac{1}{2}} \cos \psi. \quad \text{(B1b)}$$

$\gamma_1 = 1, \gamma_2 = \frac{4}{3}, K = 0$:

$$[A(\tau) - 2b][A(\tau) + b]^{\frac{1}{2}} = \left(\frac{9a}{2}\right)^{\frac{1}{2}} (\tau - \tau_0). \quad \text{(B2a)}$$

$$A(\psi) = \frac{a}{2}\psi^2 - b,$$
$$\tau - \tau_0 = \frac{a}{6}\psi^3 - b\psi. \quad \text{(B2b)}$$

$\gamma_1 = 1, \gamma_2 = \frac{4}{3}, K = +1$:

$$[A^2(\tau) + 2aA(\tau) + 2ab]^{\frac{1}{2}} - a \sinh^{-1} \frac{A(\tau) + a}{[a(a + 2b)]^{\frac{1}{2}}} = \tau - \tau_0. \quad \text{(B3a)}$$

$$A(\psi) = [a(a + 2b)]^{\frac{1}{2}} \sinh \psi - a,$$
$$\tau - \tau_0 = [a(a + 2b)]^{\frac{1}{2}} \cosh \psi - a\psi. \quad \text{(B3b)}$$

$\gamma_1 = 1, \gamma_2 = 2, K = 0$:

$$A(\tau) = \left[\frac{9a}{2}(\tau - \tau_0)^2 - b\right]^{\frac{1}{3}}. \quad \text{(B4)}$$

$\gamma_1 = \frac{4}{3}, \gamma_2 = \frac{5}{3}, K = 0$:

$$\left[A(\tau) - \frac{3b}{2}\right][A^2(\tau) + bA(\tau)]^{\frac{1}{2}} + \frac{3b^2}{4} \log \left([A^2(\tau) + bA(\tau)]^{\frac{1}{2}} + A(\tau) + \frac{b}{2}\right) = (8a)^{\frac{1}{2}}(\tau - \tau_0). \quad \text{(B5a)}$$

$$[A^2(\psi) + bA(\psi)]^{\frac{1}{2}} - \frac{b}{2} \cosh^{-1}\left[\frac{2A(\psi) + b}{b}\right] = (2a)^{\frac{1}{2}}\psi,$$
$$\tau - \tau_0 = \int A(\psi)\, d\psi. \quad \text{(B5b)}$$

$\gamma_1 = \frac{4}{3}, \gamma_2 = 2, K = -1$:

$$A(\psi) = (a + [a(a + 2b)]^{\frac{1}{2}} \sin 2\psi)^{\frac{1}{2}},$$
$$\tau - \tau_0 = \int A(\psi)\, d\psi. \quad \text{(B6)}$$

$\gamma_1 = \frac{4}{3}$, $\gamma_2 = 2$, $K = 0$:

$$A(\tau)[A^2(\tau) + b]^{\frac{1}{2}} - b \log (A(\tau) + [A^2(\tau) + b]^{\frac{1}{2}}) = (8a)^{\frac{1}{2}}(\tau - \tau_0). \quad \text{(B7a)}$$

$$A(\psi) = [2a\psi^2 - b]^{\frac{1}{2}},$$

$$\tau - \tau_0 = \frac{\psi}{2}[2a\psi^2 - b]^{\frac{1}{2}} - b\left(\frac{a}{2}\right)^{\frac{1}{2}} \log [(2a)^{\frac{1}{2}}\psi + (2a\psi^2 - b)^{\frac{1}{2}}]. \quad \text{(B7b)}$$

$\gamma_1 = \frac{4}{3}$, $\gamma_2 = 2$, $K = +1$:

$$A(\psi) = ([a(a + 2b)]^{\frac{1}{2}} \sinh 2\psi - a)^{\frac{1}{2}},$$

$$\tau - \tau_0 = \int A(\psi)\, d\psi. \quad \text{(B8)}$$

$\gamma_1 = \frac{5}{3}$, $\gamma_2 = 2$, $K = 0$:

$$[A(\tau) - b]^{\frac{1}{2}}[3A^2(\tau) - 4bA(\tau) + 8b^2] = 15\left(\frac{a}{2}\right)^{\frac{1}{2}}(\tau - \tau_0). \quad \text{(B9a)}$$

$$[A(\psi) + b]^{\frac{1}{2}}[A(\psi) - 2b] = \left(\frac{9a}{2}\right)^{\frac{1}{2}}\psi,$$

$$\tau - \tau_0 = \int A(\psi)\, d\psi. \quad \text{(B9b)}$$

APPENDIX C: THREE-COMPONENT RELATIVISTIC FLUID CASES

For Robertson–Walker cosmological models containing three noninteracting relativistic fluids each obeying an equation of state

$$p_i = (\gamma_i - 1)\mu_i, \quad i = 1, 2, 3,$$

where $\gamma_i = 1, \frac{4}{3}, \frac{5}{3}$, or 2, the solution (28) or (31a) may be readily reduced to closed form in only one case, namely, $\gamma_1 = \frac{4}{3}$, $\gamma_2 = \frac{5}{3}$, $\gamma_3 = 2$, $K = 0$. The total mass–energy density and total pressure are then

$$\mu = \frac{B_1}{A^4} + \frac{B_2}{A^5} + \frac{B_3}{A^6},$$

$$p = \frac{B_1}{3A^4} + \frac{2B_2}{3A^5} + \frac{B_3}{A^6},$$

respectively. The functions $A(\tau)$ and $A(\psi)$ are given below, using the abbreviations

$$a \equiv \kappa B_1/6, \quad b \equiv B_2/B_1, \quad c \equiv B_3/B_1.$$

Note that for $c = 0$ this solution reduces to the two-component solution (B5).

$\gamma_1 = \frac{4}{3}$, $\gamma_2 = \frac{5}{3}$, $\gamma_3 = 2$, $K = 0$:

$$\left[A(\tau) - \frac{3b}{2}\right][A^2(\tau) + bA(\tau) + c]^{\frac{1}{2}} + \left[\frac{3b^2}{4} - c\right] \times \log \left([A^2(\tau) + bA(\tau) + c]^{\frac{1}{2}} + A(\tau) + \frac{b}{2}\right) = (8a)^{\frac{1}{2}}(\tau - \tau_0). \quad \text{(C1a)}$$

$$[A^2(\psi) + bA(\psi) + c]^{\frac{1}{2}} - \frac{b}{2}\cosh^{-1}\frac{2A(\psi) + b}{[b^2 - 4c]^{\frac{1}{2}}} = (2a)^{\frac{1}{2}}\psi,$$

$$\tau - \tau_0 = \int A(\psi)\, d\psi. \quad \text{(C1b)}$$

Equations of the de Broglie Wavefield in the Case of Spherical Symmetry

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(Received 16 January 1968)

Two methods of integrating the equations of the de Broglie wavefield are introduced. The first integrating method does not seem to be as suitable for the domain of the microphysics as the second one. According to the second integrating method, the equations of the de Broglie wavefield are solved for the metric with spherical symmetry. In this case, the equations of the de Broglie wavefield admit of a solution which includes both Schrödinger and Hamilton–Jacobi methods of description as particular cases.

I. INTRODUCTION

In Riemannian space–time, one can consider the relativistic action function as a system of wave 3-surfaces of a progressive wave called in this paper the de Broglie wave. The first fundamental form of space–time represents the elementary wave 3-surfaces of such de Broglie waves and the relativistic action function, regarded as the wave 3-surface, is an envelope of these elementary wave 3-surfaces. The propagation of de Broglie waves is given by the elementary 3-surfaces which, however, are determined by the fundamental metric tensor. Thus, the fundamental metric tensor of space–time determines the propagation of de Broglie waves. Such a description of propagation is given by the homogeneous canonical system and corresponds to the original formulation of Huygens principle.[1]

However, one can attempt to describe the propagation of de Broglie waves in the spirit of Kirchhoff formulation of Huygens principle, i.e., using partial differential equations. This possibility of description seems to be given by the equations of de Broglie wavefield (briefly, field equations).[2] The field equations describe the same wavefield as the homogeneous canonical system, but from a higher analytical point of view than the homogeneous canonical system does. By an analysis of the continuation properties of the field equations, we get the equation

$$(g_{ab} - \dot{x}_a\dot{x}_b)\,dx^a\,dx^b = 0,$$

which corresponds to the local light cone and where the $\dot{x}^a \equiv dx^a/ds$ are components of the unit normal 4-vector to the wave 3-surface of the de Broglie wave.

The field equations bear no obvious resemblance to any equations of quantum mechanics. But we will establish a close connection by considering, in Sec. V, the de Broglie wavefield with spherical symmetry. Mathematically, this case is comparatively simple and the treatment is completely satisfactory. Thus, if we have confidence in the practical validity of quantum mechanics, we are in a position to compare the field equations with physical reality.

It is quite possible, however, that another case of symmetry (for example, axial symmetry) is more suitable than the case considered.

II. FIELD EQUATIONS

The field equations are[2,3]

$$R_a^b - \dot{x}_a\dot{x}^k R_k^b = (\mathcal{H}^2/h^2)(\delta_a^b - \dot{x}_a\dot{x}^b), \tag{1}$$

where $g_{ab} = g_{ba}$, $\mathcal{H}$ is the rest mass, h is Planck's constant, and $\dot{x}^a$ are components of the unit normal 4-vector to the wave 3-surface of the de Broglie wave. The system (1) is not symmetric. It can be easily rewritten in a symmetric form. Contracting (1) we get

$$R - \dot{x}^a\dot{x}^b R_{ab} = 3\mathcal{H}^2/h^2. \tag{2}$$

Multiplying (1) by $\dot{x}_b$ we have

$$R_{ab}\dot{x}^b = \dot{x}_a\dot{x}^k\dot{x}^b R_{kb}. \tag{3}$$

From (2) and (3) we obtain

$$R_{ab}\dot{x}^b = \dot{x}_a(R - 3\mathcal{H}^2/h^2). \tag{4}$$

Applying (4) we can rewrite the Eqs. (1) as

$$R_{ab} - \dot{x}_a\dot{x}_b\left(R - 3\frac{\mathcal{H}^2}{h^2}\right) = \frac{\mathcal{H}^2}{h^2}(g_{ab} - \dot{x}_a\dot{x}_b) \tag{5}$$

and, hence, after simple rearrangement on the left- and right-hand sides, we finally get

$$R_{ab} - \tfrac{1}{2}Rg_{ab} + \frac{\mathcal{H}^2}{h^2}\,g_{ab} = -\left(R - 4\frac{\mathcal{H}^2}{h^2}\right)(\tfrac{1}{2}g_{ab} - \dot{x}_a\dot{x}_b). \tag{6}$$

The systems (5), (6), and (1) are equivalent.

[1] J. Kulhanek, Nuovo Cimento **38**, 1178 (1965).
[2] J. Kulhanek, Nuovo Cimento Suppl. **4**, 172 (1966).
[3] The Eqs. (1) are introduced in Ref. 2 with a minus sign on the right-hand side. In this case, however, the solution considered in this paper does not exist. Because of this, we will consider the system (1) with a plus sign on the right-hand side as basic form of equations of de Broglie wavefield.

On the left-hand side of (6), there is a well-known tensor whose covariant divergence vanishes. Thus, from (6) we have the four conservation equations

$$g^{bl}[(R - 4\mathcal{H}^2/h^2)(\tfrac{1}{2}g_{ab} - \dot{x}_a\dot{x}_b)]_{|l} = 0. \tag{7}$$

Because

$$g^{ab}\dot{x}_a\dot{x}_b = 1 \quad \text{and hence} \quad \dot{x}^b\dot{x}_{b|a} = 0, \tag{8}$$

we find from (7) that

$$\dot{x}^l_{|l} = -\frac{1}{2}\frac{1}{R - 4\mathcal{H}^2/h^2}\frac{\partial R}{\partial x^a}\dot{x}^a. \tag{9}$$

Consequently,

$$\frac{\partial(-g)^{\frac{1}{2}}(R - 4\mathcal{H}^2/h^2)^{\frac{1}{2}}\dot{x}^a}{\partial x^a} = 0 \tag{10}$$

or

$$[(R - 4\mathcal{H}^2/h^2)^{\frac{1}{2}}\dot{x}^a]_{|a} = 0. \tag{11}$$

Thus there is a simple integral theorem

$$\oint_{V_3}\epsilon(N)\left(R - 4\frac{\mathcal{H}^2}{h^2}\right)^{\frac{1}{2}}\dot{x}_aN^a\,d_3v = 0, \tag{12}$$

with the integral taken over any closed 3-space, where N^a is its unit normal and $\epsilon(N)$ is the indicator[4] of the vector N^a. The symbol d_3v denotes an invariant element of 3-volume. The integral theorem (12) is an immediate consequence of (10). Substituting from (9) into (7), we get

$$\dot{x}^l\dot{x}_{a|l} = (\delta^l_a - \dot{x}^l\dot{x}_a)\frac{\partial}{\partial x^l}\ln\left(R - 4\frac{\mathcal{H}^2}{h^2}\right)^{\frac{1}{2}}. \tag{13}$$

The conservation equations (7) are equivalent to Eqs. (11) and (13). Let us introduce the 4-vector C_a as

$$C_a = f\dot{x}_a, \quad \text{where} \quad f = (R - 4\mathcal{H}^2/h^2)^{\frac{1}{2}}, \tag{14}$$

and the tensor[5,6] Ω_{ab} as

$$\Omega_{ab} = \frac{\partial C_b}{\partial x^a} - \frac{\partial C_a}{\partial x^b}. \tag{15}$$

Then we may rewrite (11) and (13) as

$$C^a_{|a} = 0, \quad C^a\Omega_{ab} = 0. \tag{16}$$

Thus, from (6) and (16) we may construct a system which is hyperbolic in the sense of Leray.[7,8]

Equations (1), (5), and (6) do not contain sources; hence we are dealing with continuous and nondualistic field theory. There are no reasons to distinguish between exterior and interior solutions of Eqs. (1), (5), or (6).

III. FIRST INTEGRATING METHOD

For any given set of four functions $\dot{x}_a(x^k)$, sufficiently smooth (for simplicity, let us suppose them to be of class C^2), for which we assume that

$$g^{ab}\dot{x}_a\dot{x}_b = 1, \tag{17}$$

where the g^{ab} are constructed from the g_{ab} in the usual manner, the system

$$R_{ab} - \tfrac{1}{2}Rg_{ab} + \frac{\mathcal{H}^2}{h^2}g_{ab} = -\left(R - 4\frac{\mathcal{H}^2}{h^2}\right)(\tfrac{1}{2}g_{ab} - \dot{x}_a\dot{x}_b) \tag{18}$$

is a set of ten nonlinear second-order partial differential equations to be satisfied by the ten unknowns g_{ab}. The four conservation equations

$$g^{jk}[(R - 4\mathcal{H}^2/h^2)(\tfrac{1}{2}g_{lk} - \dot{x}_l\dot{x}_k)]_{|j} = 0 \tag{19}$$

are consequences of (18) and imply no restriction on the chosen $\dot{x}_a(x^k)$, since they contain the unknowns g_{ab}, not only in the coefficients, but also in the derivatives. Since the given $\dot{x}_a(x^k)$ do not uniquely determine the coordinate system, we have to add coordinate conditions. These are only 3 in number because of (17) which represents the fourth-coordinate condition.

Example: Let us consider $\dot{x}_a(x^k)$ given as (0, 0, 0, 1). Then from (17) we obtain

$$g^{44} = 1. \tag{20}$$

Putting $g_{\alpha 4} = 0$ ($\alpha = 1, 2, 3$), from (20) we get $g_{44} = 1$. Thus we may solve (18), for example, in Gauss normal coordinates.

IV. SECOND INTEGRATING METHOD

The components of 4-vector $\dot{x}_a$ and the rest mass $\mathcal{H}$ are defined[1] as

$$\dot{x}_a = \frac{p_a}{(g^{kl}p_kp_l)^{\frac{1}{2}}}, \quad \mathcal{H} = (g^{ab}p_ap_b)^{\frac{1}{2}}, \tag{21}$$

where p_a are components of the 4-momentum. We may write[1] that

$$p_a = \frac{\partial W}{\partial x^a} \equiv W_{,a}, \tag{22}$$

where $W(x^k)$ is the covariant action function. The 3-surfaces $W = \text{const}$ are wave 3-surfaces of the de Broglie wave. Using (22) and (21) we have

$$\dot{x}_a = \frac{W_{,a}}{(g^{lk}W_{,l}W_{,k})^{\frac{1}{2}}} \equiv \frac{W_{,a}}{\mathcal{H}} \tag{23}$$

[4] For any vector V^a, the quadratic form $g_{ab}V^aV^b$ is positive, negative, or zero. If the value is not zero, we define the indicator of V^a, denoted by $\epsilon(V)$, to be ± 1 so as to make $\epsilon(V)g_{ab}V^aV^b > 0$.

[5] A. Lichnerowicz, *Recent Development in General Relativity* (Polish Scientific Publishers, Warsaw, 1962).

[6] J. L. Synge, Proc. Math. Soc. (London) **43**, 376 (1937).

[7] J. Leray, *Hyperbolic Differential Equations* (Princeton University Press, Princeton, N.J., 1951).

[8] A. Lichnerowicz, Ann. Sci. Econ. Norm. Suppl. **8**, 285 (1941).

and

$$\mathcal{K}^2 = g^{ab}W_{,a}W_{,b}. \tag{24}$$

Substituting from (23) and (24) into (6), we get

$$R_{ab} - \tfrac{1}{2}Rg_{ab} + \frac{\mathcal{K}^2}{h^2}\,g_{ab} = -\left(R - 4\frac{\mathcal{K}^2}{h^2}\right)\left(\tfrac{1}{2}g_{ab} - \frac{1}{\mathcal{K}^2}\,W_{,a}W_{,b}\right). \tag{25}$$

In (25) and (24) we have $1 + 10 = 11$ equations to be satisfied by the following 11 unknowns: g_{ab}, W. On account of a well-known argument,[9] we may consider four of the ten g_{ab} as arbitrarily given (sufficiently smooth) functions. Thus, within the condition of admissibility,[10] we have liberty in the choice of coordinates.

V. SOLUTION FOR SPHERICAL SYMMETRY

Spherical symmetry is interesting by virtue of its comparative simplicity and the physical problems associated with it. We will make our calculation for the form

$$-d\tau^2 = e^{\alpha}(dx^1)^2 + e^{\beta}[(dx^2)^2 + \sin^2 x^2(dx^3)^2] - e^{\gamma}(dx^4)^2, \tag{26}$$

where α, β, γ are three functions of (x^1, x^4).[11] For the form (26) we have

$$g_{ab} = \operatorname{diag}(e^{\alpha}, e^{\beta}, e^{\beta}\sin^2 x^2, -e^{\gamma}), \tag{27}$$

all other components vanishing and $\mathcal{K}^2 = -\mathcal{K}^2$,[12] where $\mathcal{K}$ is the rest energy of the particle. Then from (24) and (25) we have

$$-\mathcal{K}^2 = e^{-\alpha}W_{,1}^2 + e^{-\beta}[W_{,2}^2 + \sin^{-2}x^2 W_{,3}^2] - e^{-\gamma}W_{,4}^2 \tag{28}$$

and

$$R_{kk} - \tfrac{1}{2}Rg_{kk} - \frac{\mathcal{K}^2}{h^2}\,g_{kk} = -\left(R + 4\frac{\mathcal{K}^2}{h^2}\right)\left(\tfrac{1}{2}g_{kk} + \frac{1}{\mathcal{K}^2}\,W_{,k}W_{,k}\right),$$

$$R_{14} = -\left(R + 4\frac{\mathcal{K}^2}{h^2}\right)\frac{1}{\mathcal{K}^2}\,W_{,1}W_{,4}. \tag{29}$$

In the Ricci tensor, a component vanishes if it has just one subscript 2 or one subscript 3, a fact which is easy to verify without calculation on the basis of the symmetry alone. Now let us put

$$g_{22} = e^{\beta} = l^2\,(= \text{const}). \tag{30}$$

We can introduce coordinates x^1 and x^4 (isothermal coordinates)[13] such that (26) becomes

$$-d\tau^2 = e^{u}(dr^2 - dt^2) + l^2(d\vartheta^2 + \sin^2\vartheta d\phi^2) \tag{31}$$

where $r = x^1$, $\vartheta = x^2$, $\phi = x^3$, $t = x^4$, and u is a function of r, t. By direct computation under the assumption that $W_{,r} \neq 0$ and $W_{,t} \neq 0$, the Eqs. (29) give two equations

$$1 = \frac{\mathcal{K}^2}{h^2}\,l^2, \quad \frac{\partial^2 u}{\partial r^2} - \frac{\partial^2 u}{\partial t^2} = -2\frac{\mathcal{K}^2}{h^2}\,e^{u}. \tag{32}$$

From the first Eq. (32) we have

$$l^2 = h^2/\mathcal{K}^2, \quad [l] = cm, \tag{33}$$

and we identify l as Compton's wavelength. With l^2 obtained from the first equation (32), the second equation (32) gives

$$\frac{\partial^2 u}{\partial r^2} - \frac{\partial^2 u}{\partial t^2} = -\frac{2}{l^2}\,e^{u}. \tag{34}$$

Let us remark that the surface of a 2-sphere ($r = r_0 = \text{const}$) is $4\pi l^2$ for the metrics (31), which is independent of r_0. The space-time is a manifold of constant curvature $R = -4\mathcal{K}^2/h^2 = -4/l^2$ and Eq. (7), therefore, holds identically. Equation (28) now gives

$$-\mathcal{K}^2 = e^{-u}(W_{,r}^2 - W_{,t}^2) + l^{-2}(W_{,\vartheta}^2 + \sin^2\vartheta W_{,\phi}^2). \tag{35}$$

The solution of (35) is

$$W = v(r, t) + v_1(\vartheta) + v_2(\phi) \tag{36}$$

and (35) with (36) gives

$$-\mathcal{K}^2 = e^{-u}(v_{,r}^2 - v_{,t}^2) + B^2/l^2, \tag{37}$$

where B is a separation constant. The quantity $v_{,t}$ is total energy of the particle and $v_{,r}$ is its momentum. Hence, $v_{,t}^2 > v_{,r}^2$ and from (37) we see that

$$-B^2 - \mathcal{K}^2/l^2 < 0.$$

In (37) and (34) we have two differential equations,

$$u_{,rr} - u_{,tt} = -\frac{2}{l^2}\,e^{u}, \quad v_r^2 - v_{,t}^2 = -\frac{B^2 + \mathcal{K}^2 l^2}{l^2}\,e^{u}, \tag{38}$$

for two unknown functions $u(r, t)$ and $v(r, t)$. In order to solve Eqs. (38) we put

$$x = (2)^{\frac{1}{2}}r/l, \quad y = (2)^{\frac{1}{2}}t/l \tag{39}$$

[9] D. Hilbert, Ges. Wiss. Göttingen Nachr. **18**, 395 (1915).

[10] We recall from Ref. 11 the assumed existence of admissible coordinates in space-time, for which coordinates we have continuity of g_{ab} and $g_{ab,\kappa}$ across any 3-space Σ. If Σ is in some sense a 3-space of discontinuity, the discontinuity can occur only in the second or higher derivatives of g_{ab}, provided the coordinates are admissible.

[11] J. L. Synge, *Relativity: The General Theory* (North-Holland Pub. Co., Amsterdam, 1960).

[12] When the signature of first metric form is $+2$, we put $\mathcal{K}^2 = -\mathcal{K}^2$ and consider $\mathcal{K}$ as the rest mass. When the signature is -2 we put $\mathcal{K}^2 = \mathcal{K}^2$ and consider $\mathcal{K}$ as the rest mass.

[13] W. B. Bonnor, *Recent Development in General Relativity* (Polish Scientific Publishers, Warsaw, 1962).

and

$$x = \xi + \mu, \quad y = \xi - \mu. \tag{40}$$

Hence,

$$\xi = \tfrac{1}{2}(x + y), \quad \mu = \tfrac{1}{2}(x - y). \tag{41}$$

Using (39), (40), and (41), we may rewrite Eqs. (38) as

$$u_{,\xi\mu} = -e^u, \quad v_\xi v_\mu = -\tfrac{1}{2}(B^2 + \mathcal{K}^2 l^2)e^u. \tag{42}$$

The general solution of the first of Eqs. (42) is given[14] as

$$e^u = -2\frac{f'\varphi'}{(f+\varphi)^2}, \tag{43}$$

where $f(\xi)$ and $\varphi(\mu)$ are arbitrary functions. It is easy to verify that we may rewrite (43) in the form

$$e^u = -2\frac{\partial}{\partial\xi}\ln(f+\varphi)\frac{\partial}{\partial\mu}\ln(f+\varphi). \tag{44}$$

Substituting Eq. (44) in the second of Eqs. (42), we have that

$$v = (B^2 + \mathcal{K}^2 l^2)^{\frac{1}{2}} \ln(f+\varphi) \tag{45}$$

is the solution of second equation (42). Further, Eq. (43) may be written in the form

$$e^u = -\frac{1}{(f+\varphi)^2}\frac{\partial^2}{\partial\xi\,\partial\mu}(f+\varphi)^2. \tag{46}$$

Now, if we put

$$\psi = (f+\varphi)^2, \tag{47}$$

Eq. (46) then gives

$$\psi_{,\xi\mu} + e^u\psi = 0. \tag{48}$$

In the variables r, t we have (48) in the form

$$\psi_{,rr} - \psi_{,tt} + 2l^{-2}e^u\psi = 0. \tag{49}$$

With the help of (45) and (47) we may express the ψ function by means of the action function v. We obtain

$$\psi = \exp[2(B^2 + \mathcal{K}^2 l^2)^{-\frac{1}{2}}v]. \tag{50}$$

Equation (49) is the Schrödinger equation which corresponds to the Hamilton–Jacobi equation (37) and ψ is the wavefunction well known from quantum mechanics. Substituting from (50) into (48), we get

$$2(B^2 + \mathcal{K}^2 l^2)^{-1}v_\xi v_\mu + e^u + 2(B^2 + \mathcal{K}^2 l^2)^{-\frac{1}{2}} \times [(B^2 + \mathcal{K}^2 l^2)^{-\frac{1}{2}}v_\xi v_\mu - v_{\xi\mu}] = 0. \tag{51}$$

Because of (45) we may write

$$\exp[2(B^2 + \mathcal{K}^2 l^2)^{-\frac{1}{2}}v] = f(\xi) + \varphi(\mu)$$

and hence

$$\{\exp[2(B^2 + \mathcal{K}^2 l^2)^{-\frac{1}{2}}v]\}_{\xi\mu} = 0. \tag{52}$$

Owing to (52) and the second equation (42), we see that (51) holds identically. The significance of all this is that we have essentially two arbitrary functions u, v and Eqs. (42) or functions u, ψ and the equations

$$u_{rr} - u_{tt} + \frac{2}{l^2}e^u = 0, \quad \psi_{rr} - \psi_{tt} + \frac{2}{l^2}e^u\psi = 0. \tag{53}$$

Now let us assume that the function u depends only on the variable r. Then from the first equation (53) we have

$$\frac{d^2u}{dr^2} + \frac{2}{l^2}e^u = 0 \quad \text{and hence} \quad \frac{du}{dr} = \pm\frac{2}{l}(C_1 - e^u)^{\frac{1}{2}}, \tag{54}$$

where C_1 is an integration constant. The solution of (54) is given as

$$C_1 = C^2 > 0, \quad e^{-u} = C^{-2}ch^2C(rl^{-1} - C_2), \tag{55}$$

where C_2 is a second-integration constant. In this case we can assume the function ψ in the form

$$\psi = \chi(r)\Theta(t). \tag{56}$$

From the second equation (53) we get

$$\chi'' + \left(k + 2\frac{\mathcal{K}^2}{h^2}e^u\right)\chi = 0, \quad \Theta + k\Theta = 0, \tag{57}$$

where for l^2 we use (33) and k is the constant of separation. The solution of the second equation (57) is

$$\Theta = a_1\exp[(-k)^{\frac{1}{2}}t] + a_2\exp[-(-k)^{\frac{1}{2}}t], \tag{58}$$

where a_1, a_2 are integration constants. Substituting from (55) in the first equation (57), we get

$$\frac{d^2\chi}{dr^2} + \frac{2\mathcal{K}}{h^2}\left(E + \frac{V_0}{ch^2\alpha r}\right)\chi = 0, \tag{59}$$

where $E = kh^2/2\mathcal{K}$, $V_0 = \mathcal{K}C^2$, $\alpha = C\mathcal{K}/h$, and we put $C_2 = 0$. This equation is discussed in Ref. 15. The spectrum of positive eigenvalues of the energy $E = kh^2/2\mathcal{K}$ is continuous, while that of negative eigenvalues is discrete. The energy levels are determined[15] as

$$E = -\frac{h^2\alpha^2}{8\mathcal{K}}\left[-(1+2n) + \left(1 + \frac{8\mathcal{K}V_0}{\alpha^2h^2}\right)^{\frac{1}{2}}\right]^2, \tag{60}$$

where n takes positive integral values starting from zero. Substituting in (60) for V_0 and α, we get

$$E = -\tfrac{1}{2}C^2\mathcal{K}(1-n)^2. \tag{61}$$

There is a finite number of levels determined by the

[14] A. R. Forsyth, *A Treatise on Differential Equations* (Dover Publications, Inc., London, 1921), p. 555.

[15] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Addison-Wesley Publ. Co., Inc., Reading, Mass., 1958), p. 69.

condition

$$2n < \left(1 + \frac{8\mathcal{K}V_0}{\alpha^2 h^2}\right)^{\frac{1}{2}} - 1. \tag{62}$$

In our case we have

$$n < 1 \tag{63}$$

and, hence, $n = 0$. From (61) we get

$$E = -\tfrac{1}{2}C^2\mathcal{K} \quad \text{or} \quad k = -(\mathcal{K}^2/h^2)C^2. \tag{64}$$

Thus we have only one level which corresponds to number $n = 0$. Substituting k from (64) in (58), we see that ψ is not periodical in time. On the other hand, however, for $E > 0$ and hence $k > 0$ the spectrum of E is continuous and ψ is periodical in time.

VI. CONCLUSION

The solution of the field equations carried out in this paper seems to be strong support for the idea that the ψ function of quantum mechanics is in the immediate connection with the metric field of space–time.

ACKNOWLEDGMENTS

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

Analysis of Electromagnetic Radiation in the Presence of a Uniformly Moving, Uniaxially Anisotropic Medium

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(Received 7 March 1968)

The change in the character of electromagnetic radiation in the presence of a nondispersive, electrically and magnetically uniaxially anisotropic medium moving uniformly in the direction of its axis of symmetry is investigated. Because of the existing symmetry, it is possible to obtain explicit time-dependent analytic solutions for a longitudinally—and a transversely—oriented magnetic dipole current distribution density using a spectral representation in the space–time Fourier domain. The supports of the resulting fields are found to be oblate spheroidal wavefronts which enclose the source point if $v < v_1$, where v and v_1 signify respectively the speed of the medium and the phase speed of a wave, as measured by an observer in the rest frame of the material, and move inside circular conical regions—a phenomenon known as the *Čerenkov effect*—for $v > v_1$.

1. INTRODUCTION

A resurgence of interest in the subject of electrodynamics of uniformly moving media has been observed recently. The pioneering work of Minkowski[1] and Sommerfeld[2] has been used to examine the problem of electromagnetic radiation in a homogeneous, isotropic, dispersive and nondispersive, bounded and unbounded medium for both nonrelativistic and relativistic velocities.[3–29] More recently, Tai[30] investigated the first-order theory of the electrodynamics of moving anisotropic media, and Lee and Lo[31] formulated the problem of radiation in an anisotropic plasma moving along a static magnetic field. In the same vein, Chawla and Unz[32] and McKenzie[33] constructed the basic equations for a moving anisotropic plasma following the microscopic Lorentzian viewpoint.

The analysis of electromagnetic radiation arising from elementary sources in the presence of a class of "generalized" media—materials "extended" by the addition of anisotropy and motion—is the objective of this exposition. The fundamental work of Minkowski is used throughout. According to this approach, the properties of the medium, which are specified via the constitutive relations in its rest frame, are assumed to be known *a priori*. The Lorentz transformations of the theory of special relativity are then applied to write relations valid in the laboratory frame with respect to which the material is moving with uniform, but otherwise arbitrary, velocity.

It is our specific intent in this paper to examine the modification of the character of radiation in the presence of a nondispersive, both electrically and magnetically uniaxially anisotropic medium moving

condition

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It is our specific intent in this paper to examine the modification of the character of radiation in the presence of a nondispersive, both electrically and magnetically uniaxially anisotropic medium moving

uniformly along its distinguished axis. By virtue of the existing symmetry with respect to this direction, explicit solutions are found for a longitudinally—and transversely—oriented magnetic dipole by utilizing a spectral representation in the space–time Fourier domain.

2. THE MAXWELL–MINKOWSKI EQUATIONS FOR AN ANISOTROPIC MEDIUM

Consider two inertial reference frames K and K' in relative motion. The primed coordinate system is at rest with respect to a homogeneous, nondispersive, time-invariant, anisotropic medium of infinite extent, moving with a uniform velocity $\mathbf{v}$ relative to K.

In the laboratory frame the electromagnetic fields must satisfy Maxwell's curl equations

$$\nabla \times \mathbf{E} = -\partial \mathbf{B}/\partial t - \mathbf{J}_m, \tag{2.1a}$$

$$\nabla \times \mathbf{H} = \partial \mathbf{D}/\partial t + \mathbf{J}_e, \tag{2.1b}$$

where $\mathbf{J}_e$ and $\mathbf{J}_m$ are, respectively, the externally applied current distribution densities.

In the light of the Lorentz covariance, Maxwell's equations must have the same form in all inertial frames of reference. To render this set of equations closed in K', we specify the following constitutive relations:

$$\mathbf{D}' = \boldsymbol{\epsilon}' \cdot \mathbf{E}', \tag{2.2a}$$

$$\mathbf{B}' = \boldsymbol{\mu}' \cdot \mathbf{H}'. \tag{2.2b}$$

The permittivity and permeability tensors are taken to be independent of the space coordinates and time.

According to Minkowski's theory, Eqs. (2.2a) and (2.2b) suffice to determine the corresponding auxiliary relations for the unprimed field quantities if the Lorentz relativistic transformations are known.

If the coordinate frames K and K' are coincident at $t = t'$, have the same orientation, and move with a uniform velocity $\mathbf{v}$ with respect to each other, the following expressions relate the primed with the unprimed fields:

$$\mathbf{E}' = \boldsymbol{\nu} \cdot \mathbf{E} + \gamma \mathbf{v} \cdot \mathbf{B}, \tag{2.3a}$$

$$\mathbf{B}' = \boldsymbol{\nu} \cdot \mathbf{B} - (\gamma/c^2)\mathbf{v} \cdot \mathbf{E}, \tag{2.3b}$$

$$\mathbf{D}' = \boldsymbol{\nu} \cdot \mathbf{D} + (\gamma/c^2)\mathbf{v} \cdot \mathbf{H}, \tag{2.3c}$$

$$\mathbf{H}' = \boldsymbol{\nu} \cdot \mathbf{H} - \gamma \mathbf{v} \cdot \mathbf{D}, \tag{2.3d}$$

where

$$\boldsymbol{\nu} = \gamma \mathbf{I} + (1 - \gamma)v^{-2}\mathbf{v}\mathbf{v}; \quad \gamma = (1 - \beta^2)^{-\frac{1}{2}}, \quad \beta = v/c.$$

$\mathbf{I}$ is a unit dyadic or idemfactor, and the antisymmetric tensor $\mathbf{v}$ is defined so that $\mathbf{v} \cdot \mathbf{F} = \mathbf{v} \times \mathbf{F}$ for an arbitrary vector $\mathbf{F}$.

Substituting Eqs. (2.3a)–(2.3d) into Eqs. (2.2a) and (2.2b), one obtains, after a series of rearrangements,[34]

$$\mathbf{D} = \boldsymbol{\epsilon} \cdot \mathbf{E} + \boldsymbol{\xi} \cdot \mathbf{H}, \tag{2.4a}$$

$$\mathbf{B} = \boldsymbol{\zeta} \cdot \mathbf{E} + \boldsymbol{\mu} \cdot \mathbf{H}, \tag{2.4b}$$

where

$$\boldsymbol{\epsilon} = (\boldsymbol{\nu} + \gamma^2 \boldsymbol{\epsilon}' \cdot \mathbf{v} \cdot \boldsymbol{\nu}^{-1} \cdot \boldsymbol{\mu}' \cdot \mathbf{v})^{-1} \cdot [\boldsymbol{\epsilon}' \cdot \boldsymbol{\nu} + (\gamma^2/c^2)\boldsymbol{\epsilon}' \cdot \mathbf{v} \cdot \boldsymbol{\nu}^{-1} \cdot \mathbf{v}], \tag{2.5a}$$

$$\boldsymbol{\mu} = (\boldsymbol{\nu} + \gamma^2 \boldsymbol{\mu} \cdot \mathbf{v} \cdot \boldsymbol{\nu}^{-1} \cdot \boldsymbol{\epsilon}' \cdot \mathbf{v})^{-1} \cdot [\boldsymbol{\mu}' \cdot \boldsymbol{\nu} + (\gamma^2/c^2)\boldsymbol{\mu}' \cdot \mathbf{v} \cdot \boldsymbol{\nu}^{-1} \cdot \mathbf{v}], \tag{2.5b}$$

$$\boldsymbol{\xi} = -(\boldsymbol{\nu} + \gamma^2 \boldsymbol{\epsilon}' \cdot \mathbf{v} \cdot \boldsymbol{\nu}^{-1} \cdot \boldsymbol{\mu}' \cdot \mathbf{v})^{-1} \cdot [(\gamma/c^2)\mathbf{v} - \gamma \boldsymbol{\epsilon}' \cdot \mathbf{v} \cdot \boldsymbol{\nu}^{-1} \cdot \boldsymbol{\mu}' \cdot \boldsymbol{\nu}], \tag{2.5c}$$

$$\boldsymbol{\zeta} = (\boldsymbol{\nu} + \gamma^2 \boldsymbol{\mu}' \cdot \mathbf{v} \cdot \boldsymbol{\nu}^{-1} \cdot \boldsymbol{\epsilon}' \cdot \mathbf{v})^{-1} \cdot [(\gamma/c^2)\mathbf{v} - \gamma \boldsymbol{\mu}' \cdot \mathbf{v} \cdot \boldsymbol{\nu}^{-1} \cdot \boldsymbol{\epsilon}' \cdot \boldsymbol{\nu}]. \tag{2.5d}$$

The expressions for $\mathbf{D}$ and $\mathbf{B}$ [cf. Eqs. (2.4a) and (2.4b)] are introduced next into the set of Maxwell's equations in K to obtain the "definite" form

$$\mathbf{D}_\zeta \times \mathbf{E} = -(\partial/\partial t)\boldsymbol{\mu} \cdot \mathbf{H} - \mathbf{J}_m, \tag{2.6a}$$

$$\mathbf{D}_\xi \times \mathbf{H} = (\partial/\partial t)\boldsymbol{\epsilon} \cdot \mathbf{E} + \mathbf{J}_e, \tag{2.6b}$$

where the symbols $\mathbf{D}_\xi$ and $\mathbf{D}_\zeta$ represent the differential operators $\nabla - \boldsymbol{\xi}\partial/\partial t$ and $\nabla + \boldsymbol{\zeta}\partial/\partial t$, respectively. Here, $\boldsymbol{\xi}$ and $\boldsymbol{\zeta}$ are the axial vectors corresponding to

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the antisymmetric tensors ξ and ζ given in Eqs. (2.5c) and (2.5d), respectively. These relations, commonly referred to as the *Maxwell–Minkowski equations*, will be specialized in the following section to the case of a uniaxially-anisotropic medium.

3. SPECIALIZATION TO THE CASE OF A UNIAXIALLY ANISOTROPIC MEDIUM

We assume here that the material is characterized by the constitutive relations (2.2a) and (2.2b), with the electric and magnetic permittivity tensors given as

$$\epsilon' = \epsilon_1' \mathrm{I}_t + \epsilon_3' \mathbf{a}_z \mathbf{a}_z \quad \text{and} \quad \mu' = \mu_1' \mathrm{I}_t + \mu_3' \mathbf{a}_z \mathbf{a}_z,$$

respectively, in the principal-axes coordinate system.[35] This presupposes the fact that the matrix representations of the dyadic permittivities must be *semisimple* in the original coordinate system.[36]

If the velocity of the medium is directed along the axis of symmetry, i.e., $\mathbf{v} = v\mathbf{a}_z$, the constitutive relations in the K frame are found to be

$$\mathbf{D} = \epsilon \cdot \mathbf{E} + \Omega_1 \times \mathbf{H}, \tag{3.1a}$$

$$\mathbf{B} = -\Omega_1 \times \mathbf{E} + \mu \cdot \mathbf{H}, \tag{3.1b}$$

accompanied by the following definitions:

$$\begin{aligned} \epsilon &= a_1 \epsilon_1' \mathrm{I}_t + \epsilon_3' \mathbf{a}_z \mathbf{a}_z, \\ \mu &= a_1 \mu_1' \mathrm{I}_t + \mu_3' \mathbf{a}_z \mathbf{a}_z, \\ a_1 &= (1 - \beta^2)/(1 - n_1^2 \beta^2), \\ n_1 &= (\epsilon_1' \mu_1' / \epsilon_0 \mu_0)^{\frac{1}{2}}, \\ \Omega_1 &= \frac{\beta(n_1^2 - 1)}{c(1 - n_1^2 \beta^2)} \mathbf{a}_z. \end{aligned}$$

A special effort has been made to keep the notation as close as possible to that introduced earlier by other workers.

On the basis of these assumptions, the Maxwell–Minkowski set of Sec. 2 reduces now to the following simplified form:

$$\mathbf{D}_1 \times \mathbf{E} = -(\partial/\partial t)\mu \cdot \mathbf{H} - \mathbf{J}_m, \tag{3.2a}$$

$$\mathbf{D}_1 \times \mathbf{H} = (\partial/\partial t)\epsilon \cdot \mathbf{E} + \mathbf{J}_e. \tag{3.2b}$$

$\mathbf{D}_1$ designates the differential operator $\nabla - \Omega_1(\partial/\partial t)$.

4. SIX-VECTOR FORMULATION: THE RADIATION PROBLEM FOR Φ IN THE DUAL SPACE

Define Φ as an ordered pair of the vectors $\mathbf{E}$ and $\mathbf{H}$; similarly, define $\mathbf{F}$ as the ordered pair of the forcing function vectors $\mathbf{J}_e$ and $\mathbf{J}_m$, viz.,

$$\Phi = (\Phi_1, \Phi_2, \cdots, \Phi_6) = (\mathbf{E}, \mathbf{H}), \tag{4.1a}$$

$$\mathbf{F} = (F_1, F_2, \cdots, F_6) = (\mathbf{J}_e, \mathbf{J}_m). \tag{4.1b}$$

The Maxwell–Minkowski equations, as they appear in the previous section, are two separate three-vector systems for the electromagnetic field intensities $\mathbf{E}$ and $\mathbf{H}$. With the above definitions of Φ and $\mathbf{F}$, Eqs. (3.2a) and (3.2b) are converted into a single, six-vector system having the matrix representation[37]

$$\underline{C}^0 \partial \underline{\Phi}/\partial t + \underline{Q}\underline{\Phi} = -\underline{\mathbf{F}}, \tag{4.2}$$

where

$$\underline{C}^0 = \left[\begin{array}{c|c} \underline{\epsilon} & \underline{\Omega}_1 \\ \hline -\underline{\Omega}_1 & \underline{\mu} \end{array}\right], \quad \underline{Q} = \left[\begin{array}{c|c} 0 & -\underline{\mathfrak{X}} \\ \hline \underline{\mathfrak{X}} & 0 \end{array}\right],$$

$$\underline{\mathfrak{X}} = \begin{bmatrix} 0 & -\partial/\partial z & \partial/\partial y \\ \partial/\partial z & 0 & -\partial/\partial x \\ -\partial/\partial y & \partial/\partial x & 0 \end{bmatrix}.$$

Operating with the fourfold space-time Fourier transform on the inhomogeneous equation (4.2) results in

$$[\underline{Q}(\mathbf{s}) - i\omega \underline{C}^0]\underline{\Phi}(\mathbf{s}, \omega) = -\underline{\mathbf{F}}(\mathbf{s}, \omega), \tag{4.3}$$

from which

$$\underline{\Phi}(\mathbf{s}, \omega) = -[\underline{Q}(\mathbf{s}) - i\omega \underline{C}^0]^{-1} \underline{\mathbf{F}}(\mathbf{s}, \omega). \tag{4.4}$$

The matrix $\underline{Q}(\mathbf{s})$ in the dual space is given by

$$\underline{Q}(\mathbf{s}) = \left[\begin{array}{c|c} 0 & -i\underline{S} \\ \hline i\underline{S} & 0 \end{array}\right]; \quad \underline{S} = \begin{bmatrix} 0 & -s_z & s_y \\ s_z & 0 & -s_x \\ -s_y & s_x & 0 \end{bmatrix}.$$

Primarily because the velocity of the moving anisotropic medium is chosen to be along the axis of symmetry (z axis), it is allowable to write

$$\underline{Q}(\mathbf{s}) - i\omega \underline{C}^0 = \underline{\mathcal{R}}(\mathbf{s}') - i\omega \underline{\xi}, \tag{4.5}$$

[35] With $\epsilon_1' \neq \epsilon_3'$ and/or $\mu_1' \neq \mu_3'$, the medium is called uniaxially anisotropic. Often, the z' axis is referred to as the "distinguished" axis, or as the axis of symmetry of the material.

[36] M. C. Pease, III, *Methods of Matrix Algebra* (Academic Press Inc., New York, 1965), Chap. 5.

[37] Our formulation of a specific problem has led us to a system of partial differential equations [cf. Eqs. (4.2)], called the *normal* (or *canonical*) form, which has several distinct advantages. It is not only compact and suggestive, but, more importantly, it enables one to include in a single general discussion a large number of physically important problems, many of the similarities among which would be, undoubtedly, not revealed without resorting to such a systematic and unifying approach. Furthermore, most results of partial differential equations are stated in terms of the normal form. Specifically, statements concerning existence and uniqueness of solutions, and classification as to hyperbolicity, ellipticity, etc., or linearity, quasilinearity, etc., are made more conveniently in terms of the normal form.

in which

$$\underline{\mathcal{R}}(\mathbf{s}') = \begin{bmatrix} 0 & -i\underline{S}' \\ i\underline{S}' & 0 \end{bmatrix}, \quad \underline{\mathcal{E}} = \begin{bmatrix} \underline{\epsilon} & 0 \\ 0 & \underline{\mu} \end{bmatrix};$$

$$\underline{S}' = \begin{bmatrix} 0 & -s_z' & s_y' \\ s_z' & 0 & -s_x' \\ -s_y' & s_x' & 0 \end{bmatrix},$$

and $\mathbf{s}' = s_x\mathbf{a}_x + s_y\mathbf{a}_y + (s_z + \omega\Omega_1)\mathbf{a}_z$. With this transformation, the analysis of the radiation problem, at least in the dual domain, will be parallel to that for a stationary medium having the same characteristic properties. It must be emphasized, however, that this analogy is due to the particular choice of the direction of the velocity along the z axis. If, in contrast, the material moves in any other direction, the matrices $\underline{\epsilon}$ and $\underline{\mu}$ in the K inertial frame are no longer uniaxial.

With the modification shown in Eq. (4.5), one obtains

$$\underline{\Phi}(\mathbf{s}, \omega) = -[\underline{\mathcal{R}}(\mathbf{s}') - i\omega\underline{\mathcal{E}}]^{-1}\underline{\mathbf{F}}(\mathbf{s}, \omega). \tag{4.6}$$

The inverse of the matrix within the square brackets will be represented spectrally by means of a complete set of eigenvectors of $\underline{\mathcal{R}}(s')$ with $\underline{\mathcal{E}}$ in the role of a weight matrix operator. In order to accomplish this task it is mandatory that the precise nature of the eigenvalues and eigenvectors associated with this characteristic problem be investigated first.

5. PROPERTIES OF THE EIGENVALUES AND EIGENVECTORS

Consider the expression

$$\underline{\mathcal{R}}\underline{\varphi}_i = \kappa_i\underline{\mathcal{E}}\underline{\varphi}_i, \quad i = 1, 2, \cdots, 6. \tag{5.1}$$

Since both $\underline{\epsilon}$ and $\underline{\mu}$ are assumed to be real symmetric, $\underline{\mathcal{E}}^\dagger = \underline{\mathcal{E}}$. However, for real $\mathbf{s}$, $\underline{\mathcal{R}}^\dagger = -\underline{\mathcal{R}}$, i.e., $\underline{\mathcal{R}}$ is an anti-Hermitian matrix.

Theorem: The eigenvalues κ_i of $\underline{\mathcal{R}}$ are imaginary.

Theorem: The eigenvectors of (5.1) are $\underline{\mathcal{E}}$ orthogonal, viz.,[38–40]

$$\langle\underline{\varphi}_i, \underline{\mathcal{E}}\underline{\varphi}_j\rangle = T_i\delta_{ij}. \tag{5.2}$$

The proofs of both theorems are easily obtainable.

Equation (5.1) may be now recast in the form

$$\underline{\mathcal{M}}\underline{\varphi}_i = \kappa_i\underline{\varphi}_i; \quad \underline{\mathcal{M}} \equiv \underline{\mathcal{E}}^{-1}\underline{\mathcal{R}}. \tag{5.3}$$

Alternatively,

$$\underline{\mathcal{R}}\underline{\mathcal{E}}^{-1}(\underline{\mathcal{E}}\underline{\varphi}_i) = \kappa_i(\underline{\mathcal{E}}\underline{\varphi}_i) \tag{5.4}$$

is a statement of the eigenvalue problem adjoint to (5.3); namely,

$$\underline{\mathcal{M}}^\dagger\underline{\Psi}_i = \kappa_i^*\underline{\Psi}_i, \tag{5.5}$$

since $\underline{\mathcal{M}}^\dagger = -\underline{\mathcal{R}}\underline{\mathcal{E}}^{-1}$ and $\kappa_i = -\kappa_i^*$. Hence, $\underline{\Psi}_i = \underline{\mathcal{E}}\underline{\varphi}_i$. One may, therefore, substitute for (5.2) the biorthogonality condition

$$\langle\underline{\varphi}_i, \underline{\Psi}_j\rangle = T_i\delta_{ij}. \tag{5.6}$$

6. EXPANSIONS OF FUNCTIONS OF $\underline{\mathcal{M}}$ AND $\underline{\mathcal{M}}^\dagger$ IN TERMS OF $\underline{\mathcal{E}}$ DYADS AND THEIR ADJOINTS

By analogy to the outer unitary product of two vectors, the $\underline{\mathcal{E}}$ dyad $\underline{E}_{ij}$ and its adjoint $\underline{E}_{ij}^\dagger$ are defined as follows[41,42]:

$$\underline{E}_{ij} = (1/T_i)\underline{\varphi}_i\underline{\Psi}_j^\dagger, \tag{6.1a}$$

$$\underline{E}_{ij}^\dagger = (1/T_i)\underline{\Psi}_j\underline{\varphi}_i^\dagger. \tag{6.1b}$$

Four significant relationships which are required in our subsequent discussion are listed here:

$$\text{(i)} \qquad \underline{I} = \sum_{i=1}^{6}\underline{E}_{ii}, \tag{6.2a}$$

$$\text{(ii)} \qquad \underline{I} = \sum_{i=1}^{6}\underline{E}_{ii}^\dagger, \tag{6.2b}$$

$$\text{(iii)} \quad f(\underline{\mathcal{M}}) = \sum_{i=1}^{6}f(\kappa_i)\underline{E}_{ii}, \tag{6.2c}$$

$$\text{(iv)} \quad f(\underline{\mathcal{M}}^\dagger) = \sum_{i=1}^{6}f(-\kappa_i)\underline{E}_{ii}^\dagger. \tag{6.2d}$$

These relations presuppose completeness of $\{\underline{\varphi}_i\}$ and $\{\underline{\Psi}_i\}$—the set of eigenvectors of $\underline{\mathcal{M}}$ and its Hermitian adjoint $\underline{\mathcal{M}}^\dagger$. This, in turn, implies that both $\underline{\mathcal{M}}$ and $\underline{\mathcal{M}}^\dagger$ should be semisimple matrices. The validity of this assumption will be investigated in Sec. 7. In the meantime, properties (i)–(iv) will be considered valid. In relation (iii), $f(\kappa)$ is a function expressible as a power series whose radius of convergence includes all the eigenvalues of $\underline{\mathcal{M}}$. A similar statement holds for relation (iv).

Consider now the coefficient matrix appearing inside the square brackets in Eq. (4.6), viz.,

$$\underline{\Gamma} = \underline{\mathcal{R}} - i\omega\underline{\mathcal{E}} \tag{6.3a}$$

or

$$\underline{\Gamma} = \underline{\mathcal{E}}(\underline{\mathcal{M}} - i\omega\underline{I}), \tag{6.3b}$$

[38] The matrix $\underline{\mathcal{E}}$ in $\langle\underline{\varphi}_i, \underline{\mathcal{E}}\underline{\varphi}_i\rangle$ is nonsingular and Hermitian, but not necessarily positive definite. We specify that $\langle\underline{\varphi}_i, \underline{\mathcal{E}}\underline{\varphi}_i\rangle \neq 0$ in order to avoid the introduction of the concept of an "improper inner product." For further clarification, see Refs. 39 and 40.

[39] M. C. Pease, Ref. 36, pp. 215–238.

[40] W. C. Meacham, Phys. Fluids **4**, 1517 (1961).

[41] M. C. Pease, Ref. 36, Chap. 10

[42] A. D. Bresler and N. Marcuvitz, Brooklyn Polytechnic Institute, Microwave Research Institute Report No. R-565-57, 1957, Appendix I.

so that property (iii) applies. Thus,

$$\underline{\Gamma} = \sum_{i=1}^{6} (\kappa_i - i\omega)(1/T_i)\underline{\mathcal{E}}\underline{\boldsymbol{\varphi}}_i\underline{\boldsymbol{\varphi}}_i^{\dagger}\underline{\mathcal{E}}. \tag{6.3c}$$

Furthermore, the inverse of $\underline{\Gamma}$ assumes the form

$$\underline{\Gamma}^{-1} = \sum_{i=1}^{6} (\kappa_i - i\omega)^{-1}(1/T_i)\underline{\boldsymbol{\varphi}}_i\underline{\boldsymbol{\varphi}}_i^{\dagger}. \tag{6.4}$$

Equations (6.3c) and (6.4) for the expansions of $\underline{\Gamma}$ and $\underline{\Gamma}^{-1}$ can also be reached via property (iv). This, of course, necessitates writing $\underline{\Gamma}$ and $\underline{\Gamma}^{-1}$ in terms of $\underline{\mathcal{M}}^{\dagger}$, viz., $\underline{\Gamma} = (-\underline{\mathcal{M}}^{\dagger} - i\omega\underline{\mathcal{E}})\underline{\mathcal{E}}$ and

$$\underline{\Gamma}^{-1} = \underline{\mathcal{E}}^{-1}(-\underline{\mathcal{M}}^{\dagger} - i\omega\underline{I})^{-1}.$$

That $\underline{\Gamma}$ and $\underline{\Gamma}^{-1}$ given in Eqs. (6.3c) and (6.4) are, indeed, inverses of each other follows without difficulty.

7. SYNTHESIS OF SIX-EIGENVECTORS FROM TWO SETS OF THREE-EIGENVECTORS

On the strength of the transformation indicated in Eq. (4.5), we shall be able to synthesize a complete set of six-eigenvectors of the matrix $\underline{\mathcal{M}}$ from the eigenvectors of two separate three-vector problems. This, again, is possible because of the symmetry present, and should not be thought of as a general procedure.

It can be established that, corresponding to the eigenvalue problem

$$\text{(I)} \qquad \underline{S}'\underline{\mu}^{-1}\underline{S}'\underline{\mathbf{e}}_i = \lambda_i\underline{\epsilon}\underline{\mathbf{e}}_i, \tag{7.1}$$

one has the eigenvector set

$$\underline{\mathbf{e}}_1 = \underline{S}'\underline{\mathbf{a}}_z, \quad \underline{\mathbf{e}}_2 = \underline{\epsilon}^{-1}\underline{S}'\underline{S}'\underline{\mathbf{a}}_z, \quad \underline{\mathbf{e}}_3 = \underline{\mathbf{s}}'$$

and the eigenvalues

$$\lambda_1 = -[(1/a_1\mu_3'\epsilon_1')s_t'^2 + (1/a_1^2\mu_1'\epsilon_1')s_z'^2],$$
$$\lambda_2 = -[(1/a_1\mu_1'\epsilon_3')s_t'^2 + (1/a_1^2\mu_1'\epsilon_1')s_z'^2],$$
$$\lambda_3 = 0.$$

By direct analogy to these findings, given the characteristic problem

$$\text{(II)} \qquad \underline{S}'\underline{\epsilon}^{-1}\underline{S}'\underline{\mathbf{h}}_i = \chi_i\underline{\mu}\underline{\mathbf{h}}_i, \tag{7.2}$$

associated with the characteristic values

$$\chi_1 = -[(1/a_1\mu_3'\epsilon_1')s_t'^2 + (1/a_1^2\mu_1'\epsilon_1')s_z'^2],$$
$$\chi_2 = -[(1/a_1\mu_1'\epsilon_3')s_t'^2 + (1/a_1^2\mu_1\epsilon_1')s_z'^2],$$
$$\chi_3 = 0,$$

are the eigenvectors

$$\underline{\mathbf{h}}_1 = \underline{\mu}^{-1}\underline{S}'\underline{S}'\underline{\mathbf{a}}_z, \quad \underline{\mathbf{h}}_2 = \underline{S}'\underline{\mathbf{a}}_z, \quad \underline{\mathbf{h}}_3 = \underline{\mathbf{s}}'.$$

The eigenvalues and eigenvectors of the second problem have been labeled so that the eigenvectors $\underline{\mathbf{e}}_i$, $\underline{\mathbf{h}}_i$, $i = 1, 2, 3$, with the same subscript are referred to the same eigenvalue $\lambda_i = \chi_i$.[43,44]

Theorem: If, given $\underline{\mathbf{e}}_i'$ and $\underline{\mathbf{h}}_i'$, $\underline{\boldsymbol{\varphi}}_i = (\underline{\mathbf{e}}_i', \underline{\mathbf{h}}_i')$ is an eigenvector of $\underline{\mathcal{M}}$ or, equivalently, of $\underline{\mathcal{R}}$ with respect to the weight matrix $\underline{\mathcal{E}}$, corresponding to the eigenvalue κ_i, i.e.,

$$\underline{\mathcal{R}}\underline{\boldsymbol{\varphi}}_i = \kappa_i\underline{\mathcal{E}}\underline{\boldsymbol{\varphi}}_i, \tag{7.3}$$

then $\underline{\mathbf{e}}_i'$ and $\underline{\mathbf{h}}_i'$ are respectively eigenvectors of problems (I) and (II) associated with the same eigenvalue κ_i^2.[45]

Proof: If $\underline{\boldsymbol{\varphi}}_i = (\underline{\mathbf{e}}_i', \underline{\mathbf{h}}_i')$ is substituted in Eq. (7.3), by eliminating $\underline{\mathbf{e}}_i'$ first and then $\underline{\mathbf{h}}_i'$, there result the characteristic expressions

$$\underline{S}'\underline{\mu}^{-1}\underline{S}'\underline{\mathbf{e}}_i' = \kappa_i^2\underline{\epsilon}\underline{\mathbf{e}}_i', \tag{7.4a}$$

$$\underline{S}'\underline{\epsilon}^{-1}\underline{S}'\underline{\mathbf{h}}_i' = \kappa_i^2\underline{\mu}\underline{\mathbf{h}}_i', \tag{7.4b}$$

which show immediately that the eigenvalues κ_i of $\underline{\mathcal{M}}$ occur in pairs as follows:

$$\kappa_{1,4} = \pm\lambda_1^{\frac{1}{2}}, \quad \kappa_{2,5} = \pm\lambda_2^{\frac{1}{2}}, \quad \kappa_{3,6} = 0. \tag{7.5}$$

This ordering of the eigenvalues is justified by the fact that if $\underline{\boldsymbol{\varphi}}_i = (\underline{\mathbf{e}}_i', \underline{\mathbf{h}}_i')$ is an eigenvector of $\underline{\mathcal{M}}$ with the eigenvalue κ_i, then $\underline{\boldsymbol{\varphi}}_{i+3} = (\underline{\mathbf{e}}_i', -\underline{\mathbf{h}}_i')$, $i = 1, 2$, is an eigenvector of $\underline{\mathcal{M}}$ associated with $-\kappa_i$. The validity of this statement can be established without difficulty.

Consider formally the eigenvectors $\underline{\boldsymbol{\varphi}}_i = (\underline{\mathbf{e}}_i', \underline{\mathbf{h}}_i')$, $\underline{\boldsymbol{\varphi}}_{i+3} = (\underline{\mathbf{e}}_i', -\underline{\mathbf{h}}_i')$, $i = 1, 2$, $\underline{\boldsymbol{\varphi}}_3 = (\underline{\mathbf{e}}_3', 0)$, and $\underline{\boldsymbol{\varphi}}_6 = (0, \underline{\mathbf{h}}_3')$. All that is known about this set is that it satisfies the eigenvalue problem (7.3). In addition to this requirement, however, it is necessary that it also obey the biorthogonality condition and the completeness relationships.

We shall examine next the implications of these restrictions. First it is specified that

$$\langle\underline{\boldsymbol{\varphi}}_i, \underline{\boldsymbol{\psi}}_j\rangle = 0, \quad i \neq j. \tag{7.6}$$

The only difficulty with reference to this condition arises from the eigenvectors $\underline{\boldsymbol{\varphi}}_i$ and $\underline{\boldsymbol{\varphi}}_{i+3}$, $i = 1, 2$. More specifically,

$$\langle\underline{\boldsymbol{\varphi}}_i, \underline{\boldsymbol{\psi}}_{i+3}\rangle = N_i' - M_i' = 0, \quad i = 1, 2, \tag{7.7}$$

where $N_i' = \langle\underline{\mathbf{e}}_i', \underline{\mathbf{d}}_i'\rangle$, $M_i' = \langle\underline{\mathbf{h}}_i', \underline{\mathbf{b}}_i'\rangle$ and $\underline{\mathbf{d}}_i' = \underline{\epsilon}\underline{\mathbf{e}}_i'$,

[43] G. A. Deschamps and O. B. Kesler, Trans. IEEE Antennas Propagation **12**, 783 (1964).

[44] O. B. Kesler, thesis, University of Illinois, 1965, Chap. 5.

[45] The prime signifies that $\underline{\mathbf{e}}_i'$ and $\underline{\mathbf{h}}_i'$ are suitably chosen scalar multiples of $\underline{\mathbf{e}}_i$ and $\underline{\mathbf{h}}_i$ satisfying the biorthogonality condition $\langle\underline{\boldsymbol{\varphi}}_i, \underline{\boldsymbol{\psi}}_j\rangle = 0$, $i \neq j$. This point will be discussed in greater detail again later in this section.

$\underline{\mathbf{b}}'_i = \underline{\mu}\underline{\mathbf{h}}'_i$. Since the two terms on the right-hand side cannot vanish individually, it follows that the sets $\{\underline{\mathbf{e}}'_i\}$ and $\{\underline{\mathbf{h}}'_i\}$ must be constructed so that $N'_i = M'_i$, $i = 1, 2$.

Theorem: The eigenvector sets $\{\underline{\mathbf{e}}'_i\}$ and $\{\underline{\mathbf{h}}'_i\}$, in the sense defined in this section, satisfy the completeness relations

$$\underline{I} = \sum_{i=1}^{3} (1/N'_i)\underline{\mathbf{e}}'_i\underline{\mathbf{d}}'^{\dagger}_i, \quad \underline{I} = \sum_{i=1}^{3} (1/M'_i)\underline{\mathbf{h}}'_i\underline{\mathbf{b}}'^{\dagger}_i. \tag{7.8}$$

The proof of the theorem follows easily since the primed eigenvectors are scalar multiples of the unprimed ones.

Theorem: The six-eigenvector sets $\{\underline{\varphi}_i\}$ and $\{\underline{\psi}_i\}$ satisfy the completeness relation

$$\underline{I} = \sum_{i=1}^{6} \underline{E}_{ii} = \sum_{i=1}^{6} (1/T_i)\underline{\varphi}_i\underline{\psi}^{\dagger}_i. \tag{7.9}$$

Proof:

$$\sum_{i=1}^{6} \underline{E}_{ii} = \sum_{j=1}^{2}[(1/T_j)\underline{\varphi}_j\underline{\psi}^{\dagger}_j + (1/T_{j+3})\underline{\varphi}_{j+3}\underline{\psi}^{\dagger}_{j+3}] + (1/T_3)\underline{\varphi}_3\underline{\psi}^{\dagger}_3 + (1/T_6)\underline{\varphi}_6\underline{\psi}^{\dagger}_6. \tag{7.10a}$$

However, $T_j = T_{j+3} = 2N'_j$, $j = 1, 2$, and $T_3 = N'_3$, $T_6 = M'_3$. Hence,

$$\sum_{i=1}^{6} \underline{E}_{ii} = \begin{bmatrix} \sum_{i=1}^{3}(1/N'_i)\underline{\mathbf{e}}'_i\underline{\mathbf{d}}'^{\dagger}_i & 0 \\ 0 & \sum_{i=1}^{3}(1/M'_i)\underline{\mathbf{h}}'_i\underline{\mathbf{b}}'^{\dagger}_i \end{bmatrix} = \underline{I}. \tag{7.10b}$$

We conclude this section with an explicit representation of the set $\{\underline{\varphi}_i\}$:

$$\underline{\varphi}_i = (\underline{\mathbf{e}}'_i, \underline{\mathbf{h}}'_i), \quad \underline{\varphi}_{i+3} = (\underline{\mathbf{e}}'_i, -\underline{\mathbf{h}}'_i), \quad i = 1, 2,$$
$$\underline{\varphi}_3 = (\underline{\mathbf{e}}'_3, 0), \quad \underline{\varphi}_6 = (0, \underline{\mathbf{h}}'_3)$$

with

$$\underline{\mathbf{e}}'_1 = |\underline{\mathbf{s}}''|\,\underline{S}'\underline{\mathbf{a}}_z, \quad \underline{\mathbf{e}}'_2 = \underline{\epsilon}^{-1}\underline{S}'\underline{S}'\underline{\mathbf{a}}_z, \quad \underline{\mathbf{e}}'_3 = \underline{\mathbf{s}}',$$

and

$$\underline{\mathbf{h}}'_1 = \underline{\mu}^{-1}\underline{S}'\underline{S}'\underline{\mathbf{a}}_z, \quad \underline{\mathbf{h}}'_2 = |\underline{\mathbf{s}}''|\,\underline{S}'\underline{\mathbf{a}}_z, \quad \underline{\mathbf{h}}'_3 = \underline{\mathbf{s}}',$$

in which

$$\mathbf{s}'' = (\mu'_3\epsilon'_1 a_1)^{-\frac{1}{2}}(s'_x\mathbf{a}_x + s'_y\mathbf{a}_y) + a_1^{-1}(\mu'_1\epsilon'_1)^{-\frac{1}{2}}s'_z\mathbf{a}_z.$$

8. SPECTRAL REPRESENTATIONS IN TERMS OF SIX- AND THREE-EIGENVECTORS

With the expansion of $\underline{\Gamma}^{-1}$ presented in Sec. 6, the field vector $\underline{\Phi}$ in Eq. (4.6) becomes

$$\underline{\Phi}(\mathbf{s}, \omega) = -\sum_{i=1}^{6} (\kappa_i - i\omega)^{-1}(1/T_i)\underline{\varphi}_i\underline{\varphi}^{\dagger}_i\underline{\mathbf{F}}(\mathbf{s}, \omega). \tag{8.1}$$

A premultiplication of both sides by $\underline{\mathcal{E}}$ results in a representation for the adjoint vector $\underline{\Psi}$:

$$\underline{\Psi}(\mathbf{s}, \omega) = -\sum_{i=1}^{6} (\kappa_i - i\omega)^{-1}\underline{E}^{\dagger}_{ii}\underline{\mathbf{F}}(\mathbf{s}, \omega) \tag{8.2}$$

or

$$\underline{\Psi}_i(\mathbf{s}, \omega) = -(\kappa_i - i\omega)^{-1}\underline{\mathbf{F}}_i(\mathbf{s}, \omega), \tag{8.3}$$

since

$$\underline{\Psi}_i(\mathbf{s}, \omega) = \underline{E}^{\dagger}_{ii}\underline{\Psi}(\mathbf{s}, \omega), \quad \underline{\mathbf{F}}_i(\mathbf{s}, \omega) = \underline{E}^{\dagger}_{ii}\underline{\mathbf{F}}(\mathbf{s}, \omega). \tag{8.4}$$

In the space–time domain,

$$\underline{\Psi} = \underline{G}(\mathbf{r}, t) * \underline{\mathbf{F}}(\mathbf{r}, t), \tag{8.5}$$

where[46]

$$\underline{G}(\mathbf{r}, t) = -\mathcal{F}_4^{-1} \cdot \left[\sum_{i=1}^{6} (\kappa_i - i\omega)^{-1}(1/T_i)\underline{\psi}_i\underline{\varphi}^{\dagger}_i\right] \tag{8.6}$$

is the matrix representation of the dyadic Green's function of the problem under consideration.

In the previous section we succeeded in constructing a complete biorthogonal six-eigenvector set out of two three-eigenvector sets. Here we shall reverse the procedure and show that the spectral resolution of $\underline{\Psi}(\mathbf{s}', \omega)$ in (8.2) leads to a representation of $\underline{\epsilon}\underline{\mathbf{E}}$ in terms of $\{\underline{\mathbf{e}}_i\}$, and $\underline{\mu}\mathbf{H}$ in terms of $\{\underline{\mathbf{h}}_i\}$. More specifically,

$$\underline{\Psi}(\mathbf{s}, \omega) = -\begin{bmatrix} \sum_{i=1}^{3}(\kappa_i^2 + \omega^2)^{-1}(1/N_i)\underline{\mathbf{d}}_i\underline{\mathbf{e}}^{\dagger}_i & 0 \\ 0 & \sum_{i=1}^{3}(\kappa_i^2 + \omega^2)(1/M_i)\underline{\mathbf{b}}_i\underline{\mathbf{h}}^{\dagger}_i \end{bmatrix}\begin{bmatrix} \underline{\mathbf{M}}_e \\ \underline{\mathbf{M}}_m \end{bmatrix}, \tag{8.7}$$

whence[47]

$$\underline{\epsilon}\underline{\mathbf{E}} \equiv \underline{\tilde{\mathbf{D}}} = -\sum_{i=1}^{3} (\lambda_i + \omega^2)^{-1}(1/N_i)\underline{\mathbf{d}}_i\underline{\mathbf{e}}^{\dagger}_i\underline{\mathbf{M}}_e, \tag{8.8a}$$

$$\underline{\mu}\mathbf{H} \equiv \underline{\tilde{\mathbf{B}}} = -\sum_{i=1}^{3} (\lambda_i + \omega^2)^{-1}(1/M_i)\underline{\mathbf{b}}_i\underline{\mathbf{h}}^{\dagger}_i\underline{\mathbf{M}}_m. \tag{8.8b}$$

The effective forcing functions are given by

$$\underline{\mathbf{M}}_e(\mathbf{s}', \omega) = i\omega\underline{\mathbf{J}}_e - i\underline{S}'\underline{\mu}^{-1}\underline{\mathbf{J}}_m, \tag{8.9a}$$

$$\underline{\mathbf{M}}_m(\mathbf{s}', \omega) = i\omega\underline{\mathbf{J}}_m + i\underline{S}'\underline{\epsilon}^{-1}\underline{\mathbf{J}}_e. \tag{8.9b}$$

It should be noted that for a moving medium, in the laboratory frame, $\underline{\epsilon}\underline{\mathbf{E}}$ represents only a part of the electric displacement, and $\underline{\mu}\mathbf{H}$ only a part of the

[46] Here (*) denotes space–time convolution, whereas $\mathcal{F}_4^{-1}$ stands for the inverse fourfold space–time Fourier transform.

[47] O. B. Kesler, Ref. 44, Chap. 3.

magnetic induction; hence the above definitions of the quantities $\underline{\tilde{\mathbf{D}}}$ and $\underline{\tilde{\mathbf{B}}}$.

One may arrive at the three-vector spectral representations exhibited in Eqs. (8.8a) and (8.8b) directly by eliminating $\underline{\mathbf{E}}$ and $\underline{\mathbf{H}}$ from the original set of the Maxwell–Minkowski equations and proceeding along parallel lines. We chose, instead, to reach them via a more general six-vector formulation.

9. THE CASE OF A LONGITUDINAL MAGNETIC DIPOLE

We undertake here the task of determining the radiation arising from a z-directed magnetic point dipole described by the current density distribution

$$\mathbf{J}_m = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t')\mathbf{a}_z. \tag{9.1}$$

The effective forcing function $\underline{\mathbf{M}}_e$ appearing in the spectral representation of $\underline{\tilde{\mathbf{D}}}$ [cf. Eq. (8.8a)] is then

$$\mathbf{M}_e(\mathbf{r}, t) = -\delta(t - t')(1/\mu_3')\nabla\delta(\mathbf{r} - \mathbf{r}') \times \mathbf{a}_z \tag{9.2}$$

in the space–time domain, and, from Eq. (8.9a), $\underline{\mathbf{M}}_e(\mathbf{s}', \omega)$ has the form

$$\underline{\mathbf{M}}_e(\mathbf{s}', \omega) = -(i/\mu_3')\underline{S}'\underline{\mathbf{a}}_z \times \exp(-i\mathbf{s}\cdot\mathbf{r}' + i\omega t') = \underline{\mathbf{M}}_{e1}(\mathbf{s}, \omega) \tag{9.3}$$

in the dual space. Since it turns out that only the component of $\underline{\mathbf{M}}_e(\mathbf{s}', \omega)$ along $\underline{\mathbf{d}}_1$ is present, a longitudinal magnetic dipole excites only the first mode; namely,

$$\underline{\tilde{\mathbf{D}}}(\mathbf{r}, t) = [\mathcal{F}_3^{-1}\cdot I_1(\mathbf{s}, t)] * [\mathcal{F}_4^{-1}\cdot(-\underline{\mathbf{M}}_{e1})]. \tag{9.4}$$

In this equation,

$$\begin{aligned} I_1(\mathbf{s}, t) &= \mathcal{F}_0^{-1}\cdot(\lambda_1 + \omega^2)^{-1} \\ &= 0, && t < 0, \\ &= a_1\epsilon_1'\mu_1'u_1^2\exp(-i\omega_0 t)(\sin\omega_1 t/\omega_1), && t > 0, \end{aligned} \tag{9.5}$$

with

$$\begin{aligned} \omega_0 &= u_1^2 s_z(\Omega_1/a_1), \\ \omega_1 &= u_1[(\mu_1'/\mu_3')s_t'^2 + b^2 s_z^2]^{\frac{1}{2}}, \\ u_1^{-2} &= a_1\epsilon_1'\mu_1' - \Omega_1^2/a_1, \\ b^2 &= a_1^{-1} + u_1^2(\Omega_1^2/a_1^2). \end{aligned}$$

The inverse spatial Fourier transform of $I_1(\mathbf{s}, t)$ is given by

$$I_2(\mathbf{r}, t) \equiv \mathcal{F}_3^{-1}\cdot I_1(\mathbf{s}, t) = 0 \tag{9.6a}$$

for $t < 0$ and

$$I_2(\mathbf{r}, t) = a_1 b\mu_3'\epsilon_1'(u_1/4\pi r_1)\delta(u_1 t - r_1) \tag{9.6b}$$

for $t \geq 0$, where

$$\mathbf{r}_1 = x_1\mathbf{a}_x + x_2\mathbf{a}_y + (x_3 - \gamma' t)\mathbf{a}_z; \quad \gamma' = u_1^2 b\Omega_1/a_1$$

and

$$\underline{\mathbf{r}}_0 = \underline{A}^{-1}\underline{\mathbf{r}}; \quad \mathbf{r}_0 = \sum_{j=1}^{3} x_j\mathbf{a}_j,$$

with

$$\underline{A} = \begin{bmatrix} (\mu_1'/\mu_3')^{\frac{1}{2}} & 0 & 0 \\ 0 & (\mu_1'/\mu_3')^{\frac{1}{2}} & 0 \\ 0 & 0 & 1/b \end{bmatrix}.$$

The inversion of the second portion of Eq. (9.4) yields

$$\mathbf{I}_3 = \mathcal{F}_4^{-1}\cdot(-\mathbf{M}_{e1}) = (i/\mu_3')\delta(t - t')\nabla\delta(\mathbf{r} - \mathbf{r}') \times \mathbf{a}_z. \tag{9.7}$$

Therefore, finally,

$$\begin{aligned} \tilde{\mathbf{D}}_1(\mathbf{r}, t) &= I_2(\mathbf{r}, t) * \mathbf{I}_3(\mathbf{r}, t) \\ &= \nabla \times [a_1\epsilon_1' b(u_1/4\pi R_1)\delta(u_1\tau - R_1)]\mathbf{a}_z, \end{aligned} \tag{9.8}$$

in which $\tau = t - t'$ and

$$R_1 = \left\{\frac{\mu_3'}{\mu_1'}[(x - x')^2 + (y - y')^2] + \frac{n_1^2 - \beta^2}{n_1^2(1 - \beta^2)}\left[z - z' - \frac{v(n_1^2 - 1)}{n_1^2 - \beta^2}\right]^2\right\}^{\frac{1}{2}}.$$

We distinguish the following two cases: If $n_1\beta < 1$, i.e., if the speed of the medium is smaller than that of propagation of light along the x axis of the material, the wavefronts, which, for constant τ, are ellipsoids with semiaxes $\tau(\mu_3'\epsilon_1')^{-\frac{1}{2}}$, $\tau(\mu_3'\epsilon_1')^{-\frac{1}{2}}$, and $\tau b^{-1}(\mu_1'\epsilon_1')^{-\frac{1}{2}}$ along the principal axes, enclose the source point resulting in what we shall, henceforth, call *ordinary radiation*. On the other hand, however, for $n_1\beta > 1$, the wavefront surfaces expand and move inside a conical region, thus giving rise to the Čerenkov effect.

By an analogous procedure, it is found that a longitudinal electric dipole excites only the second mode. The above discussion applies here unaltered except that the wavefronts now are oblate spheroids with semiaxes $\tau(\epsilon_3'\mu_1')^{-\frac{1}{2}}$, $\tau(\epsilon_3'\mu_1')^{-\frac{1}{2}}$, and $\tau b^{-1}(\epsilon_1'\mu_1')^{-\frac{1}{2}}$, that is, they are dual to the previously found ones.

These two distinct types of radiation have been referred to in the literature as the *ordinary* and *extraordinary waves*, respectively. This is due primarily to the fact that, in working with stationary uniaxially-anisotropic media, the magnetic permittivity is usually assumed to be a scalar quantity. Since, however, in this exposition, both waves are "extraordinary" in the sense that neither corresponds to a spherical wavefront, we shall no longer adhere to the established nomenclature; instead we shall refer to them as waves of type I and II, respectively.

The conical regions within which the Čerenkov phenomenon occurs for the two types of waves, although of the same general orientation, do not have in

general identical half angles. We shall return to this point in the next section where the radiation emanating from a transversely oriented magnetic dipole is examined.

10. THE CASE OF A TRANSVERSELY ORIENTED MAGNETIC DIPOLE

The illustration of the general formalism is continued in this section by examining the radiation emanating from an x-directed magnetic dipole which is described mathematically by the current density distribution

$$\mathbf{J}_m(\mathbf{r}, t) = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t')\mathbf{a}_x. \tag{10.1}$$

Since the source is not aligned with the axis of symmetry of the medium, one would, in general, expect the excitation and, consequently, the coupling of at least two modes. Of course, the matter is settled immediately by expanding the effective source function $\underline{\mathbf{M}}_e(\mathbf{s}, \omega)$ in terms of the eigenvectors $\{\underline{\mathbf{d}}_i\}$.

Corresponding to the prescribed current-density distribution in Eq. (10.1), one has the effective source function

$$\mathbf{M}_e(\mathbf{r}, t) = -\delta(t - t')\nabla \times \mu^{-1} \cdot \delta(\mathbf{r} - \mathbf{r}')\mathbf{a}_x \tag{10.2}$$

in the space–time domain, and, from Eq. (8.9a),

$$\underline{\mathbf{M}}_e(\mathbf{s}', \omega) = -(i/a_1\mu_1')\underline{S}'\underline{\mathbf{a}}_x \exp(-i\mathbf{s} \cdot \mathbf{r}' + i\omega t') \tag{10.3}$$

in the dual space. The components of $\underline{\mathbf{M}}_e(\mathbf{s}', \omega)$ along the "adjoint" eigenvectors $\underline{\mathbf{d}}_i$, $i = 1, 2, 3$, are given by

$$\underline{\mathbf{M}}_{ei} = (1/N_i)\underline{\mathbf{d}}_i\underline{\mathbf{e}}_i^{\dagger}\underline{\mathbf{M}}_e, \quad i = 1, 2, 3. \tag{10.4}$$

Specifically,

$$\underline{\mathbf{M}}_{e1}(\mathbf{s}, \omega) = (i/a_1\mu_1')(s_x's_z'/s_t'^2)\underline{S}'\underline{\mathbf{a}}_z \times \exp(-i\mathbf{s} \cdot \mathbf{r}' + i\omega t'), \tag{10.5a}$$

$$\underline{\mathbf{M}}_{e2}(\mathbf{s}, \omega) = -(i/a_1\mu_1')(s_y'/s_t'^2)\underline{S}'\underline{S}'\underline{\mathbf{a}}_z \times \exp(-i\mathbf{s} \cdot \mathbf{r}' + i\omega t'), \tag{10.5b}$$

$$\underline{\mathbf{M}}_{e3}(\mathbf{s}, \omega) = 0. \tag{10.5c}$$

It is seen, therefore, that the total field $\tilde{\underline{\mathbf{D}}}$ will consist of a combination of waves of types I and II. The spectral representation in Eq. (8.8a) enables one to find each mode separately.

The individual modes $\tilde{\underline{\mathbf{D}}}_1$ and $\tilde{\underline{\mathbf{D}}}_2$ are written as follows:

$$\tilde{\underline{\mathbf{D}}}_1(\mathbf{r}, t) = \mathcal{F}_0^{-1} \cdot \{[-\mathcal{F}_3^{-1} \cdot I^{(1)}(\mathbf{s}, \omega)] * [\mathcal{F}_3^{-1} \cdot \underline{\mathbf{I}}_1^{(1)}(\mathbf{s}, \omega)]\}, \tag{10.6a}$$

$$\tilde{\underline{\mathbf{D}}}_2(\mathbf{r}, t) = -\mathcal{F}_0^{-1} \cdot \{[-\mathcal{F}_3^{-1} \cdot I^{(2)}(\mathbf{s}, \omega)] * [\mathcal{F}_3^{-1} \cdot \underline{\mathbf{I}}_1^{(2)}(\mathbf{s}, \omega)]\} \tag{10.6b}$$

in space–time. The functions $I^{(i)}$, $\underline{\mathbf{I}}_1^{(i)}$, $i = 1, 2$, are to some extent arbitrary. Their choice, however, should be made judiciously in order that the task of carrying out the integrations be less formidable. Suppose that

$$I^{(1)}(\mathbf{s}, \omega) = (\lambda_1 + \omega^2)^{-1}s_x's_t'^{-2}, \tag{10.7a}$$

$$I^{(2)}(\mathbf{s}, \omega) = (\lambda_2 + \omega^2)^{-1}s_y's_t'^{-2}, \tag{10.7b}$$

$$\underline{\mathbf{I}}_1^{(1)}(\mathbf{s}, \omega) = (i/a_1\mu_1')s_z'\underline{S}'\underline{\mathbf{a}}_z \exp(-i\mathbf{s} \cdot \mathbf{r}' + i\omega t'), \tag{10.7c}$$

$$\underline{\mathbf{I}}_1^{(2)}(\mathbf{s}, \omega) = (i/a_1\mu_1')\underline{S}'\underline{S}'\underline{\mathbf{a}}_z \exp(-i\mathbf{s} \cdot \mathbf{r}' + i\omega t'). \tag{10.7d}$$

With this selection, the second parts in the right-hand sides of Eqs. (10.6a) and (10.6b) can be integrated out without too much difficulty. Actually,

$$\mathbf{I}_3^{(1)}(\mathbf{r}, \omega) \equiv \mathcal{F}_3^{-1} \cdot \mathbf{I}_1^{(1)}(\mathbf{s}, \omega) = (1/a_1\mu_1') \times \exp(i\omega t')[-i(\partial/\partial z)\nabla' + \omega\Omega_1\nabla']\delta(\mathbf{r} - \mathbf{r}') \times \mathbf{a}_z \tag{10.8a}$$

and

$$\mathbf{I}_3^{(2)}(\mathbf{r}, \omega) \equiv \mathcal{F}_3^{-1} \cdot \mathbf{I}_1^{(2)}(\mathbf{s}, \omega) = -(i/a_1\mu_1')\exp(i\omega t')\nabla' \times \nabla' \times \delta(\mathbf{r} - \mathbf{r}')\mathbf{a}_z. \tag{10.8b}$$

The differential operator ∇' is defined as

$$\nabla' = \mathbf{a}_x(\partial/\partial x) + \mathbf{a}_y(\partial/\partial y) + \mathbf{a}_z(\partial/\partial z + i\omega\Omega_1).$$

The first parts on the right-hand sides of Eqs. (10.6a) and (10.6b) can be written down explicitly as follows:

$$I_2^{(1)}(\mathbf{r}, \omega) \equiv -\mathcal{F}_3^{-1} \cdot I_1^{(1)}(\mathbf{s}, \omega) = \frac{a_1\mu_1'\epsilon_1'}{(2\pi)^3}\int_{E_3} \exp(i\mathbf{s} \cdot \mathbf{r}) \cdot \left[\frac{\mu_1'}{\mu_3'}s_t^2 + \frac{1}{a_1}(s_z + \omega\Omega_1)^2 - a_1\mu_1'\epsilon_1'\omega^2\right]^{-1} s_x s_t^{-2}\, d\mathbf{s}, \tag{10.9a}$$

$$I_2^{(1)}(\mathbf{r}, \omega) = -\mathcal{F}_3^{-1} \cdot I_1^{(2)}(\mathbf{s}, \omega) = \frac{a_1\mu_1'\epsilon_1'}{(2\pi)^3}\int_{E_3} \exp(i\mathbf{s} \cdot \mathbf{r}) \cdot \left[\frac{\epsilon_1'}{\epsilon_3'}s_t^2 + \frac{1}{a_1}(s_z + \omega\Omega_1)^2 - a_1\mu_1'\epsilon_1'\omega^2\right]^{-1} s_y s_t^{-2}\, d\mathbf{s}. \tag{10.9b}$$

It remains now to carry out these integrations. Since the elements of $\underline{\epsilon}'$ and $\underline{\mu}'$ are positive real numbers by hypothesis, any difficulty which may arise in performing the integrations will be due entirely to the sign of a_1 which is positive for $n_1\beta < 1$ and negative for $n_1\beta > 1$. It is imperative, therefore, that we differentiate between these two cases.

Case (i): $n_1\beta < 1$. To avoid disrupting the continuity of the main theme of this section by an excessive amount of details, we shall present here the final forms of the integrals (10.9a) and (10.9b), and include the highlights of the derivations in the Appendix:

$$I_2^{(1)}(\mathbf{r}, \omega) = \frac{ia_1(\epsilon_1'\mu_1')^{\frac{1}{2}}}{4\pi} \frac{e^{-i\omega\Omega_1 z}}{i\omega} \frac{x}{x^2 + y^2} \times [\exp(ik_0 r_1) - \exp(ik_0 a_1^{\frac{1}{2}}|z|)], \quad (10.10a)$$

$$I_2^{(2)}(\mathbf{r}, \omega) = \frac{ia_1(\epsilon_1'\mu_1')^{\frac{1}{2}}}{4\pi} \frac{e^{-i\omega\Omega_1 z}}{i\omega} \frac{y}{x^2 + y^2} \times [\exp(ik_0 r_2) - \exp(ik_0 a_1^{\frac{1}{2}}|z|)], \quad (10.10b)$$

where

$$k_0 = \omega(\epsilon_1'\mu_1')^{\frac{1}{2}},$$
$$r_1 = [(\mu_3'/\mu_1')(x^2 + y^2) + a_1 z^2]^{\frac{1}{2}},$$
$$r_2 = [(\epsilon_3'/\epsilon_1')(x^2 + y^2) + a_1 z^2]^{\frac{1}{2}}.$$

It is interesting to observe that $I_2^{(2)}$ can be obtained from $I_2^{(1)}$ by replacing x with y and substituting $\underline{\mu}'$ for $\underline{\epsilon}'$, and vice versa. Henceforth, $I_2^{(i)}$, $i = 1, 2$, will be considered as dual quantities in the sense described above.

If it is born in mind that the convolution is a commutative operation, and that $Lu = L\delta * u$ for an arbitrary differential operator and a suitable function u, it develops that

$$\tilde{\mathbf{D}}_1(\mathbf{r}, \omega) = I_2^{(1)}(\mathbf{r}, \omega) * \mathbf{I}_3^{(1)}(\mathbf{r}, \omega) = \frac{1}{4\pi}\left(\frac{\epsilon_1'}{\mu_1'}\right)^{\frac{1}{2}} e^{i\omega t'}\left(-i\frac{\partial}{\partial z}\nabla' + \omega\Omega_1\nabla'\right) \times \mathbf{a}_z \frac{e^{-i\omega\Omega_1 Z}}{\omega} \frac{X}{X^2 + Y^2} \times [\exp(ik_0 R_1) - \exp(ik_0 a_1^{\frac{1}{2}}|Z|)] \quad (10.11a)$$

and

$$\tilde{\mathbf{D}}_2(\mathbf{r}, \omega) = I_2^{(2)}(\mathbf{r}, \omega) * \mathbf{I}_3^{(2)}(\mathbf{r}, \omega) = -\frac{1}{4\pi}\left(\frac{\epsilon_1'}{\mu_1'}\right)^{\frac{1}{2}} e^{i\omega t'}\nabla' \times \nabla' \times \mathbf{a}_z \times \frac{e^{-i\omega\Omega_1 Z}}{i\omega} \frac{Y}{X^2 + Y^2} \times [\exp(ik_0 R_2) - \exp(ik_0 a_1^{\frac{1}{2}}|Z|)], \quad (10.11b)$$

where now $X = x - x'$, $Y = y - y'$, $Z = z - z'$, and

$$R_1 = [(\mu_3'/\mu_1')(X^2 + Y^2) + a_1 Z^2]^{\frac{1}{2}},$$
$$R_2 = [(\epsilon_3'/\epsilon_1')(X^2 + Y^2) + a_1 Z^2]^{\frac{1}{2}}.$$

A distinctive feature in Eqs. (10.11a) and (10.11b) is the appearance of terms proportional to

$$\exp(ik_0 a_1^{\frac{1}{2}}|Z|)$$

besides the usual factors proportional to $\exp(ik_0 R_i)$, $i = 1, 2$, after the indicated differentiations have been carried out. This feature, however, is characteristic of the individual modes, but not of the total field. The separate fields associated with $\tilde{\mathbf{D}}_1$ and $\tilde{\mathbf{D}}_2$ are connected with current distributions on the plane $Z = 0$, which have singularities at the source point, and spread over the entire plane when thought of as surface currents.[48]

We present now the fields $\tilde{\mathbf{D}}_1$ and $\tilde{\mathbf{D}}_2$ in space–time:

$$\tilde{\mathbf{D}}_1(\mathbf{r}, t) = \frac{1}{4\pi}\left(\frac{\epsilon_1'}{\mu_1'}\right)^{\frac{1}{2}}\nabla' \times \mathbf{a}_z\left\{\frac{X}{X^2 + Y^2} \times \left[a_1(a_1\epsilon_1'\mu_1')^{\frac{1}{2}}\frac{Z}{R_1}\right]\delta[\tau + \Omega_1 Z - (a_1\epsilon_1'\mu_1')^{\frac{1}{2}}R_1]\right\}, \quad (10.12)$$

$$\tilde{\mathbf{D}}_2(\mathbf{r}, t) = -\frac{1}{4\pi}\left(\frac{\epsilon_1'}{\mu_1'}\right)^{\frac{1}{2}} a_1(a_1\epsilon_1'\mu_1')^{\frac{1}{2}}\left\{\left[\nabla_t\left(\frac{Y}{X^2 + Y^2}\frac{Z}{R_2}\right) - \frac{\epsilon_3'}{\epsilon_1'}\frac{Y}{X^2 + Y^2}\mathbf{a}_z\left(\frac{\partial}{\partial x}X + \frac{\partial}{\partial y}Y\right)\frac{1}{R_2}\right] \times \delta[\tau + \Omega_1 Z - (a_1\epsilon_1'\mu_1')^{\frac{1}{2}}R_2]\right\}. \quad (10.13)$$

The support of the fields are two impulsive wavefronts which correspond to waves of type I and II, respectively. Their mathematical description is found by setting the arguments of the Dirac δ function in Eqs. (10.12) and (10.13) equal to zero, viz.,

$$\text{(i)} \quad \tau + \Omega_1 Z - (a_1\epsilon_1'\mu_1')^{\frac{1}{2}}R_1 = 0, \quad (10.14a)$$

$$\text{(ii)} \quad \tau + \Omega_1 Z - (a_1\epsilon_1'\mu_1')^{\frac{1}{2}}R_2 = 0. \quad (10.14b)$$

These expressions appear to be of a different form compared with previously encountered wavefront equations. They can, nonetheless, be converted into the standard ellipsoidal formulas[49]

$$(X^2 + Y^2)/A_i^2 + (Z - Z_c)^2/B^2 = 1, \quad i = 1, 2, \quad (10.15)$$

with

$$A_1 = [(\mu_1'/\mu_3')(1 - \beta^2)/(n_1^2 - \beta^2)]^{\frac{1}{2}}c\tau,$$
$$A_2 = [(\epsilon_1'/\epsilon_3')(1 - \beta^2)/(n_1^2 - \beta^2)]^{\frac{1}{2}}c\tau,$$
$$B = n_1 c\tau(1 - \beta^2)/(n_1^2 - \beta^2),$$
$$Z_c = \beta c\tau(n_1^2 - 1)/(n_1^2 - \beta^2).$$

An observer at an arbitrary field point will experience, in this case, the effect of two distinct impulses.

[48] P. C. Clemmow, Proc. IEEE **110**, 107 (1963).

[49] A similar conversion has been carried out by Tai (cf. Ref. 22) for a moving isotropic medium.

Case (ii): $n_1\beta > 1$. It is shown in the Appendix that

$$I_2^{(1)}(\mathbf{r}, \omega) = \frac{ia_1'(\epsilon_1'\mu_1')^{\frac{1}{2}}}{2\pi} \frac{\exp(i\omega\Omega_1' z)}{\omega} \frac{x}{x^2 + y^2} \times (\sin q_0 r_1' - \sin q_0 a_1'^{\frac{1}{2}} |z|) \quad (10.16a)$$

for $a_1'^{\frac{1}{2}} z > [(\mu_3'/\mu_1')(x^2 + y^2)]^{\frac{1}{2}}$, and

$$I_2^{(2)}(\mathbf{r}, \omega) = \frac{ia_1'(\epsilon_1'\mu_1')^{\frac{1}{2}}}{2\pi} \frac{\exp(i\omega\Omega_1' z)}{\omega} \frac{y}{x^2 + y^2} \times (\sin q_0 r_2' - \sin q_0 a_1'^{\frac{1}{2}} |z|) \quad (10.16b)$$

for $a_1'^{\frac{1}{2}} z > [(\epsilon_3'/\epsilon_1')(x^2 + y^2)]^{\frac{1}{2}}$. Both $I_2^{(1)}$ and $I_2^{(2)}$ vanish outside these regions. The following notational definitions have been used:

$$a_1' = -a_1, \quad \Omega_1' = -\Omega_1, \quad q_0 = \omega(a_1'\epsilon_1'\mu_1')^{\frac{1}{2}},$$
$$r_1' = [a_1' z^2 - (\mu_3'/\mu_1')(x^2 + y^2)]^{\frac{1}{2}},$$
$$r_2' = [a_1' z^2 - (\epsilon_3'/\epsilon_1')(x^2 + y^2)]^{\frac{1}{2}}.$$

The fields $\tilde{\mathbf{D}}_1$ and $\tilde{\mathbf{D}}_2$ in space–time are identical with these in Eqs. (10.12) and (10.13), except that R_1 and R_2 must be replaced by

$$R_1' = [a_1' Z^2 - (\mu_3'/\mu_1')(X^2 + Y^2)]^{\frac{1}{2}},$$
$$R_2' = [a_1 Z^2 - (\epsilon_3'/\epsilon_1')(X^2 + Y^2)]^{\frac{1}{2}},$$

respectively. In addition, the supports of the fields are now the impulsive wavefronts

$$\text{(i)} \quad \tau - \Omega_1' Z - (a_1'\epsilon_1'\mu_1')^{\frac{1}{2}} R_1' = 0, \quad (10.17a)$$
$$\text{(ii)} \quad \tau - \Omega_1' Z - (a_1'\epsilon_1'\mu_1')^{\frac{1}{2}} R_2 = 0, \quad (10.17b)$$

which may also be rewritten as in Eq. (10.15).

In conclusion, the range of validity of the solutions in Eqs. (10.16a) and (10.16b) is a strikingly clear mathematical evidence of the Čerenkov effect which occurs in two conical regions in this example. Although these regions (corresponding to waves of type I and II) are of the same orientation—they have a common vertex at the source point and their common axis is parallel to the z axis—they do not have the same half angles, unless $\epsilon_3'/\epsilon_1' = \mu_3'/\mu_1'$.

The entire space, therefore, can be divided into three parts: (a) the region outside both cones where no radiation fields are present; (b) the part between the inner and the outer cones where a wave of one type only can exist; and (c) the intersection of both cones which, of course, coincides with the inner or smaller cone in this case, where an interaction of both modes takes place.

11. CONCLUDING REMARKS

If the uniaxial medium is in motion with a uniform velocity directed along, say, the x axis, i.e., $\mathbf{v} = v\mathbf{a}_x$, it can be shown that the dyadics $\boldsymbol{\epsilon}$ and $\boldsymbol{\mu}$ have a diagonal form in the unprimed coordinate frame. This is a direct consequence of the choice of the motion along one of the principal axes. However, because the motion does not take place along the axis of symmetry of the medium, both $\boldsymbol{\epsilon}$ and $\boldsymbol{\mu}$ have now a biaxial character; that is, their diagonal elements are, in general, distinct.[50] In other words, apart from the intensification of the degree of anisotropy, a change in the type of anisotropy has also occurred. The tensors $\boldsymbol{\xi}$ and $\boldsymbol{\zeta}$ (see Sec. 2) are transpose with respect to each other.

In the case of the "effectively" biaxially anisotropic material described above, although it is possible to determine the eigenvalues of $\underline{\mathcal{M}}(\mathbf{s})$ (cf. Sec. 8) explicitly, and, formally, find a complete set of eigenvectors which can be used as a basis, the exact evaluation of the integrals, if not altogether impossible, can be achieved with great difficulty because of the complicated form of the eigenvalues and eigenvectors. This is, in turn, due to the involved nature of the resulting dispersion or wave-normal surface.[51]

In light of the biaxially anisotropic nature of the medium as seen by an observer in the laboratory frame, it is no longer expected that z-directed electric and magnetic dipoles give rise only to one type of radiation field, nor should it be expected the conical regions within which the Cerenkov effect occurs will be circular any longer.

ACKNOWLEDGMENTS

The author wishes to express his gratitude to Professor R. E. Collin for his advice and guidance. He is also indebted to Professor R. T. Compton, Jr., for his encouragement and helpful suggestions.

This work was supported in part by the Air Force Cambridge Research Laboratories, Office of Aerospace Research, under Contract AF19(628)-1699, while the author was at Case Institute of Technology.

APPENDIX

In this appendix we provide an outline of the steps followed in the transition from Eqs. (10.9) to (10.10), on the one hand, and from Eqs. (10.9) to (10.16), on

[50] In the nonrelativistic limit, $\boldsymbol{\epsilon} = \boldsymbol{\epsilon}'$ and $\boldsymbol{\mu} = \boldsymbol{\mu}'$; that is, the medium presents to an observer in the laboratory frame a uniaxial character, even if the motion is not in the direction of the axis of symmetry.

[51] For a stationary, biaxially anisotropic medium, the wave-normal surface is a quartic or a fourth-degree surface, symmetric with respect to the origin, and not factorable into irreducible terms of lower order. The latter is a characteristic property of both a *bona fide* uniaxially anisotropic medium whose dispersion surface is reducible to two second-order surfaces, and an isotropic medium the fourth-degree wave-normal surface of which is twofold degenerate, that is, it can be written as a product of two identical second-order factors.

the other hand, accordingly as a_1 is positive or negative.

Case (i): $n_1\beta < 1$. In Eq. (10.9a) let $\mathbf{s}$ and $\mathbf{r}$ undergo an affine transformation which takes $\underline{s}$ to $\underline{s}_0 = \underline{\underline{A}}\underline{s} + \underline{l}$ and $\underline{r}$ to $\underline{r}_0 = \underline{\underline{A}}^{-1}\underline{r}$ with

$$\underline{\underline{A}} = \begin{bmatrix} (\mu_1'/\mu_3')^{\frac{1}{2}} & 0 & 0 \\ 0 & (\mu_1'/\mu_3')^{\frac{1}{2}} & 0 \\ 0 & 0 & (1/a_1)^{\frac{1}{2}} \end{bmatrix}, \quad \underline{l} = \begin{bmatrix} 0 \\ 0 \\ \omega\Omega_1 a_1^{-\frac{1}{2}} \end{bmatrix}$$

and[31,52]

$$\mathbf{r}_0 = \sum_{i=1}^{3} \mathbf{a}_i x_i, \quad \mathbf{s}_0 = \sum_{i=1}^{3} \mathbf{a}_i s_i.$$

Under this transformation,

$$I_2^{(1)}(\mathbf{r}, \omega) = a_1^{\frac{3}{2}}\epsilon_1'(\mu_1'\mu_3')^{\frac{1}{2}} e^{-i\mathbf{l}\cdot\mathbf{r}_0} \frac{1}{(2\pi)^3} \times \int_{E_3} e^{i\mathbf{s}_0\cdot\mathbf{r}_0}(s_0^2 - k_0^2)^{-1} s_1 s_{0t}^{-2}\, d\mathbf{s}_0. \quad \text{(A1)}$$

The presence of the terms s_1 and s_{0t}^2 suggests a further transformation of the variables s_i and x_i, $i = 1, 2, 3$, into cylindrical coordinates, viz.,

$$s_1 = \rho\cos\psi, \quad s_2 = \rho\sin\psi, \quad s_3 = s_3,$$
$$x_1 = \chi\cos\alpha, \quad x_2 = \chi\sin\alpha, \quad x_3 = x_3.$$

Written in terms of the new variables, Eq. (A1) assumes the form

$$I_2^{(1)}(\mathbf{r}, \omega) = a_1^{\frac{3}{2}}\epsilon_1'(\mu_1'\mu_3')^{\frac{1}{2}} e^{-i\mathbf{l}\cdot\mathbf{r}_0} \frac{1}{(2\pi)^3} \times \int_0^{\infty}\int_{-\infty}^{\infty}\int_0^{2\pi} (\rho^2 + s_3^2 - k_0^2)^{-1} \cdots \exp i[\rho\chi\cos(\psi - \alpha) + x_3 s_3] \times \cos\psi\, d\psi\, ds_3\, d\rho. \quad \text{(A2)}$$

The integration over the variables χ and s_3 can be carried out without encountering any particular difficulty:

$$\int_0^{2\pi} \cos\psi \exp[i\rho\chi\cos(\psi - \alpha)]\, d\psi = 2\pi i J_1(\rho\chi)\cos\alpha, \quad \text{(A3)}$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{is_3 x_3}(s_3^2 + \rho^2 - k_0^2)^{-1}\, ds_3 = \frac{\exp[-|x_3|(\rho^2 - k_0^2)^{\frac{1}{2}}]}{2(\rho^2 - k_0^2)^{\frac{1}{2}}}. \quad \text{(A4)}$$

If the last two results are substituted back into Eq. (A2), one has

$$I_2^{(1)}(\mathbf{r}, \omega) = a_1^{\frac{3}{2}}\epsilon_1'(\mu_1'\mu_3')^{\frac{1}{2}} e^{-i\mathbf{l}\cdot\mathbf{r}_0} \frac{i}{4\pi}\cos\alpha \times \int_0^{\infty} J_1(\rho\chi) \frac{\exp[-|x_3|(\rho^2 - k_0^2)^{\frac{1}{2}}]}{(\rho^2 - k_0^2)^{\frac{1}{2}}}\, d\rho. \quad \text{(A5)}$$

[52] G. Birckhoff and S. MacLane, *A Brief Survey of Modern Algebra* (The Macmillan Co., New York, 1962), pp. 212, 254.

The integration over ρ can be effected with the aid of the well-known Sommerfeld formula

$$\int_0^{\infty} J_0(\nu\rho) \frac{\exp[-|x_3|(\rho^2 - k_0^2)^{\frac{1}{2}}]}{(\rho^2 - k_0^2)^{\frac{1}{2}}} \rho\, d\rho = \frac{\exp[ik_0(\nu^2 + x_3^2)^{\frac{1}{2}}]}{(\nu^2 + x_3^2)^{\frac{1}{2}}}. \quad \text{(A6)}$$

Let us multiply both sides of this equation by ν and integrate over ν from 0 to χ.[48] If, furthermore, the relation

$$\rho\int_0^{\chi} J_0(\nu\rho)\nu\, d\nu = \chi J_1(\chi\rho) \quad \text{(A7)}$$

is taken into account, it follows that

$$\int_0^{\infty} J_1(\chi\rho) \frac{\exp[-|x_3|(\rho^2 - k_0^2)^{\frac{1}{2}}]}{(\rho^2 - k_0^2)^{\frac{1}{2}}} d\rho = \frac{1}{\chi}\int_0^{\chi} \frac{\exp[ik_0(\nu^2 + x_3^2)^{\frac{1}{2}}]}{(\nu^2 + x_3^2)^{\frac{1}{2}}} \nu\, d\nu. \quad \text{(A8)}$$

The integration in the right-hand side can be completed by a simple variable substitution. Finally, in terms of the original variables,

$$I_2^{(1)}(\mathbf{r}, \omega) = \frac{ia_1(\epsilon_1'\mu_1')^{\frac{1}{2}}}{4\pi} \frac{e^{-i\omega\Omega_1 z}}{i\omega} \frac{x}{x^2 + y^2} \times [\exp(ik_0 r_1) - \exp(ik_0 a_1^{\frac{1}{2}}|z|)]. \quad \text{(A9)}$$

The function $I_2^{(2)}(\mathbf{r}, \omega)$ is the dual of $I_2^{(1)}(\mathbf{r}, \omega)$ with respect to x, y, $\underline{\epsilon}'$, and $\underline{\mu}'$.

Case (ii): $n_1\beta > 1$. Through the affine transformation $\underline{s}_0 = \underline{\underline{A}}\underline{s} + \underline{l}$ and $\underline{r}_0 = \underline{\underline{A}}^{-1}\underline{r}$ in which $\underline{\underline{A}}$ and $\underline{l}$ are prescribed as

$$\underline{\underline{A}} = \begin{bmatrix} (\mu_1'/\mu_3')^{\frac{1}{2}} & 0 & 0 \\ 0 & (\mu_1'/\mu_3')^{\frac{1}{2}} & 0 \\ 0 & 0 & (1/a_1')^{\frac{1}{2}} \end{bmatrix},$$

$$\underline{l} = \begin{bmatrix} 0 \\ 0 \\ -\omega\Omega_1' a_1'^{-\frac{1}{2}} \end{bmatrix},$$

$$a_1' = -a_1, \quad \Omega_1' = -\Omega_1,$$

and

$$\mathbf{s}_0 = \sum_{i=1}^{3} \mathbf{a}_i s_i, \quad \mathbf{r}_0 = \sum_{i=1}^{3} \mathbf{a}_i x_i,$$

one has

$$I_2^{(1)}(\mathbf{r}, \omega) = -a_1'^{\frac{3}{2}}\epsilon_1'(\mu_1'/\mu_3')^{\frac{1}{2}} e^{-i\mathbf{l}\cdot\mathbf{r}_0} \frac{1}{(2\pi)^3} \times \int_{E_3} e^{i\mathbf{s}_0\cdot\mathbf{r}_0}(s_{0t}^2 - s_3^2 + q_0^2)^{-1} s_1 s_{0t}^{-2}\, d\mathbf{s}_0. \quad \text{(A10)}$$

Resorting next exactly to the same transformation to cylindrical coordinates as in Case (i), we may write

$$I_2^{(1)}(\mathbf{r}, \omega) = -a_1'^{\frac{3}{2}}\epsilon_1'(\mu_1'/\mu_3')^{\frac{1}{2}}e^{-i\mathbf{l}\cdot\mathbf{r}_0}\frac{1}{(2\pi)^3} \times \int_0^\infty \int_{-\infty}^\infty \int_0^{2\pi} (\rho^2 - s_3^2 + q_0^2)^{-1} \times \exp i[\rho\chi\cos(\psi - \alpha) + x_3 s_3] \times \cos\psi \, d\psi \, ds_3 \, d\rho. \quad \text{(A11)}$$

The integration over the azimuthal variable ψ is the same as before [cf. Eq. (A3)]. However,

$$\frac{1}{2\pi}\int_{-\infty}^\infty e^{is_3x_3}[s_3^2 - (\rho^2 + q_0^2)]^{-1} \, ds_3 = -\frac{\sin x_3(\rho^2 + q_0^2)^{\frac{1}{2}}}{(\rho^2 + q_0^2)^{\frac{1}{2}}}, \quad x_3 > 0. \quad \text{(A12)}$$

The integral vanishes otherwise. The last integration is evaluated by means of a contour integration in the complex s_3 plane.

There still remains the integration over the variable ρ:

$$I_2^{(1)}(\mathbf{r}, \omega) = -a_1'^{\frac{3}{2}}\epsilon_1'(\mu_1'\mu_3')^{\frac{1}{2}}e^{-i\mathbf{l}\cdot\mathbf{r}_0}\frac{i}{2\pi}\cos\alpha \times \int_0^\infty J_1(\rho\chi)\frac{\sin x_3(\rho^2 + q_0^2)^{\frac{1}{2}}}{(\rho^2 + q_0^2)^{\frac{1}{2}}} \, d\rho \quad \text{(A13)}$$

for $x_3 > 0$. $I_2^{(1)}(\mathbf{r}, \omega)$ vanishes for $x_3 < 0$. Consider now the tabulated Hankel integral transform

$$\int_0^\infty J_0(\nu\rho)\frac{\sin x_3(\rho^2 + q_0^2)^{\frac{1}{2}}}{(\rho^2 + q_0^2)^{\frac{1}{2}}}\rho \, d\rho = \frac{\cos q_0(x_3^2 - \nu^2)^{\frac{1}{2}}}{(x_3^2 - \nu^2)^{\frac{1}{2}}} \quad \text{(A14)}$$

for $\nu < x_3$. This integral vanishes otherwise.[53] If, again, both sides of this relation are multiplied by ν and integrated over ν from 0 to χ,

$$\int_0^\infty J_1(\chi\rho)\frac{\sin x_3(\rho^2 + q_0^2)^{\frac{1}{2}}}{(\rho^2 + q_0^2)^{\frac{1}{2}}} \, d\rho = \frac{1}{\chi}\int_0^\chi \frac{\cos q_0(x_3^2 - \nu^2)^{\frac{1}{2}}}{(x_3^2 - \nu^2)^{\frac{1}{2}}}\nu \, d\nu, \quad \nu < x_3, \quad \text{(A15)}$$

the right-hand side of which is readily integrable.

Finally,

$$I_2^{(1)}(\mathbf{r}, \omega) = \frac{ia_1'(\epsilon_1'\mu_1')^{\frac{1}{2}}}{2\pi}\frac{e^{i\omega\Omega_1'z}}{\omega}\frac{x}{x^2 + y^2} \times (\sin q_0 r_1' - \sin q_0 a_1'^{\frac{1}{2}}|z|) \quad \text{(A16)}$$

in the region $a_1'^{\frac{1}{2}}z > [(\mu_3'/\mu_1')(x^2 + y^2)]^{\frac{1}{2}}$. The function $I_2^{(2)}(\mathbf{r}, \omega)$ is the dual of $I_2^{(1)}(r, \omega)$ in the sense mentioned earlier.

[53] A. Erdélyi, Ed., *Tables of Integral Transforms* (McGraw-Hill Book Co., New York, 1954), Vol. II.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

Generalized Bose Operators in the Fock Space of a Single Bose Operator

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(Received 2 August 1968)

Generalized Bose operators b which reduce by two the number of quanta of a Bose operator a are studied in the Fock space of a. All representations of the b's as normal-ordered (infinite degree) power series of the a's are found. The unitary operators relating the irreducible components of b to a are also exhibited. The analogous result for $b^{(k)}$'s which reduce the number of a quanta by k is given and the limit $k \to \infty$ is discussed.

I. INTRODUCTION

Free fields and canonical quantization are important in quantum theory. Besides describing the motion of noninteracting systems, these quantization methods allow treatment of in and out fields for theories with interaction and of fields for quasiparticle excitations. From the mathematical point of view, free and canonical fields can be used to construct more complicated fields; for example, in the neutrino theory of light[1] and in the theory of superconductivity.[2] Few exact explicit results are available for fields whose representation in terms of a free or canonical field contains terms of arbitrarily high degree. Several theorems state that only infinite-degree series in a free field can give nontrivial theories.[3]

In the present article, we study a very simple problem leading to infinite degree series, but we try to give a thorough treatment. Our original stimulus was the article of Streit,[4] in which unitary equivalence properties of representations of the inhomogeneous Lorentz group are used to establish the existence of generalized free fields in the Fock space of an irreducible free field.[5] We plan to study the power-series representations of such generalized free fields in a later publication. In the present article we study generalized Bose operators, which we define (in analogy to generalized free fields) to be operators whose commutator is a c-number and whose annihilation part annihilates the vacuum state, in the Fock space of a Bose operator.

After a review of the theory of a single Bose operator a in Sec. II, we define in Sec. III generalized Bose operators b which reduce the number of a quanta by two. We consider both irreducible and reducible b's and consider the unitary equivalence between the irreducible b's and the a's. In Sec. IV, we find representations of the b's as infinite-degree power series in a and a^*, valid on the domain spanned by the eigenvectors of the number operator N of the a's. This representation then determines b on its full domain by closure. We find power-series representations of b and b^* directly from their Bose commutation relations and, independently, using the relation (which we derive) $N = 2b^*b + \Lambda_-$, where Λ_- is the projector onto the odd-quanta subspace $\mathcal{H}_-$ of the a Fock space $\mathcal{H}$.[6] We show in Sec. V that the representations of b found in Sec. IV are the most general power-series representations. We construct the unitary operators $U_\pm$ relating the irreducible $b_\pm$ and a in Sec. VI. In Sec. VII, we show that the algebra $\mathcal{A}_+$ of even powers of a and a^* is irreducible, and we represent the irreducible b_+, which acts on the even-quanta subspace $\mathcal{H}_+$ of $\mathcal{H}$, as a power series in $\mathcal{A}_+$. In Sec. VIII, we give the power series for a reducible $b^{(k)}$ which reduces the number of a quanta by k and discuss the limit $k \to \infty$. Finally, we make some concluding remarks in Sec. IX.

II. REVIEW OF THEORY OF A SINGLE BOSE OPERATOR

We consider the Hilbert space $\mathcal{H}$ of sequences $\psi = \{c_n \mid n = 0, 1, 2, \cdots\}$ such that $\sum |c_n|^2 < \infty$, with the usual inner product, etc. We write

$$\psi = \sum c_n |n\rangle,$$

with $\{|n\rangle \mid n = 0, 1, 2, \cdots\}$ a complete orthonormal

* Supported in part by the U.S. Air Force Office of Scientific Research under Grant AFOSR 68-1453.
† Supported in part by the National Science Foundation under Grant NSF GP 6036.

[1] See A. S. Wightman, in *High Energy Electromagnetic Interactions and Field Theory*, M. Lèvy, Ed. (Gordon & Breach, Science Publishers, Inc., New York, 1966), and references therein.

[2] See, for example, J. Bardeen, L. N. Cooper, and J. R. Schreiffer, Phys. Rev. **108**, 1175 (1957).

[3] See, for example, K. Bardakci and E. C. G. Sudarshan, Nuovo Cimento **21**, 722 (1961); O. W. Greenberg, J. Math. Phys. **3**, 31 (1962); O. W. Greenberg and A. L. Licht, *ibid.* **4**, 613 (1963).

[4] L. Streit, Helv. Phys. Acta **39**, 65 (1965).

[5] Such generalized free fields are equivalent to infinite-degree normal-ordered series in the irreducible free fields. No finite-degree series will suffice to give a c-number commutator, since if the highest degree term has degree N, then the commutator will contain a normal-ordered term of degree $2N - 2$ which cannot be canceled by any other term.

[6] Another derivation has been given by A. L. Licht (private communication) in terms of the projection operator $|0\rangle\langle 0|$.

basis of $\mathcal{H}$:

$$\langle n \mid n' \rangle = \delta_{nn'}.$$

We define the usual annihilation operator a on this basis by

$$a\,|n\rangle = n^{\frac{1}{2}}\,|n-1\rangle, \quad n > 0, \quad a\,|0\rangle = 0.$$

The unique closure of a is given by[7]

$$a\psi = \sum (n)^{\frac{1}{2}} c_n\,|n-1\rangle$$

on its domain

$$\mathfrak{D}_a = \{\sum c_n\,|n\rangle \mid \sum |c_n|^2\, n < \infty\}.$$

The adjoint a^* of a satisfies

$$a^*\,|n\rangle = (n+1)^{\frac{1}{2}}\,|n+1\rangle$$

and the domain of its closure is also $\mathfrak{D}_a$. Thus, the number operator

$$N = a^*a$$

satisfies

$$N\,|n\rangle = n\,|n\rangle$$

and its closure has domain

$$\mathfrak{D}_N = \{\sum c_n\,|n\rangle \mid \sum |c_n|^2\, n^2 < \infty\}.$$

On $\mathfrak{D}_N$, the commutation relation

$$[a, a^*] = 1 \tag{1}$$

is valid so that $(a, \mathcal{H})$ is a representation of the abstract commutation relation corresponding to (1). This representation is irreducible and any other irreducible representation of (1) by closed densely-defined operators on a Hilbert space is unitarily equivalent to it.[8]

We note finally that the relations

$$[N, a] = -a, \quad [N, a^*] = a^* \tag{2}$$

are valid on a suitable domain.

III. GENERALIZED BOSE OPERATORS WHICH CREATE AND DESTROY TWO a QUANTA

We consider the subspace

$$\mathcal{H}_+ = \left\{\sum_{n=0}^{\infty} c_{2n}\,|2n\rangle \in \mathcal{H}\right\}$$

of $\mathcal{H}$ and define on it the operator b_+ by

$$b_+\,|2n\rangle = e^{i\theta_{2n-2}}(n)^{\frac{1}{2}}\,|2n-2\rangle, \quad b_+\,|0\rangle = 0, \tag{3}$$

with θ_{2i}, $i = 0, 1, 2, \cdots$, arbitrary real numbers. Then,

$$b_+^*\,|2n\rangle = e^{-i\theta_{2n}}(n+1)^{\frac{1}{2}}\,|2n+2\rangle \tag{4}$$

and the closure of b_+ has domain $\mathfrak{D}_a \cap \mathcal{H}_+$. We see immediately that

$$N_+ = b_+^* b_+$$

has domain $\mathfrak{D}_N \cap \mathcal{H}_+$ and satisfies there $N = 2N_+$. On $\mathfrak{D}_N \cap \mathcal{H}_+$, the commutation relation

$$[b_+, b_+^*] = 1$$

is valid so that $(b_+, \mathcal{H}_+)$ is another representation of (1). Since $(b_+, \mathcal{H}_+)$ is isomorphic to $(a, \mathcal{H})$ under $a \leftrightarrow b_+$, $|n\rangle \leftrightarrow |2n\rangle$, it is, in fact, another irreducible representation of (1).

Similarly, we can consider the subspace

$$\mathcal{H}_- = \left\{\sum_{n=0}^{\infty} c_{2n+1}\,|2n+1\rangle \in \mathcal{H}\right\}$$

of $\mathcal{H}$ and the operator b_- on $\mathcal{H}_-$ defined by

$$b_-\,|2n+1\rangle = e^{i\theta_{2n-1}}(n)^{\frac{1}{2}}\,|2n-1\rangle, \quad b_-\,|1\rangle = 0, \tag{5}$$

with θ_{2i+1}, $i = 0, 1, 2, \cdots$, again arbitrary real numbers. Then

$$b_-^*\,|2n+1\rangle = e^{-i\theta_{2n+1}}(n+1)^{\frac{1}{2}}\,|2n+3\rangle. \tag{6}$$

The closure of b_- has domain $\mathfrak{D}_a \cap \mathcal{H}_-$ and

$$N_- = b_-^* b_-$$

has domain $\mathfrak{D}_N \cap \mathcal{H}_-$ and satisfies there $N = 2N_- + 1$. On $\mathfrak{D}_N \cap \mathcal{H}_-$ the commutation relation

$$[b_-, b_-^*] = 1$$

is valid so that, since $(b_-, \mathcal{H}_-)$ is isomorphic to $(a, \mathcal{H})$, $(b_-, \mathcal{H}_-)$ is another irreducible representation of (1).

The irreducible representations $(b_\pm, \mathcal{H}_\pm)$ of (1) possess vacuum states $|\kappa_\pm\rangle$, where $\kappa_+ = 0$, $\kappa_- = 1$, and there exist unitary operators $U_\pm$ on $\mathcal{H}$ such that

$$U_\pm \mathcal{H} = \mathcal{H}_\pm \tag{7}$$

and

$$U_\pm^{-1} b_\pm U_\pm = a. \tag{8}$$

Explicitly, we can take

$$U_\pm\,|n\rangle = |2n + \kappa_\pm\rangle.$$

Now $\mathcal{H}$ is the direct sum

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-.$$

Writing $\Lambda_\pm$ as the projection operator onto $\mathcal{H}_\pm$, we

[7] See C. R. Putnam, *Commutation Properties of Hilbert Space Operators* (Springer-Verlag, Berlin, 1967), Lemma 4.43. This book contains references to the original literature.

[8] See Ref. 7, Theorem 4.5.1. This theorem requires a more precise statement of the conditions needed for uniqueness. Our operators always satisfy these conditions.

define an operator b on $\mathcal{H}$ by

$$b = b_+\Lambda_+ + b_-\Lambda_-. \tag{9}$$

Then, the closure of b has domain $\mathfrak{D}_a$ and the closure of

$$M = b^*b = N_+\Lambda_+ + N_-\Lambda_-$$

has domain $\mathfrak{D}_N$ and there satisfies

$$N = 2M + \Lambda_-.$$

The commutation relation

$$[b, b^*] = 1$$

is valid on $\mathfrak{D}_N$ so that $(b, \mathcal{H})$ is a reducible representation of (1) with irreducible decomposition (9).

Let us write the above $b_\pm$ defined by (3) and (5) as $b_\pm(\theta_\pm)$, where $\theta_\pm$ is symbolic for the set $\{\theta_i \mid i = 2j + \kappa_\pm; j = 0, 1, 2, \cdots\}$. Then if $\theta'_\pm$ are any other sets of real numbers, the corresponding $b_\pm(\theta'_\pm) \equiv b'_\pm$ also define irreducible representations of (1). Thus there exist unitary operators

$$U_\pm(\theta_\pm, \theta'_\pm), \quad U_\pm^{-1}(\theta_\pm, \theta'_\pm) = U_\pm(\theta'_\pm, \theta_\pm),$$

such that

$$U_\pm(\theta_\pm, \theta'_\pm)b_\pm(\theta'_\pm)U_\pm(\theta'_\pm, \theta_\pm) = b_\pm(\theta_\pm). \tag{10}$$

If $V_\pm(r; \alpha_r)$ are the unitary operators inducing the transformation $b_\pm(\theta_\pm) \to b_\pm(\theta_\pm^{(r)})$, with

$$\theta_i^{(r)} = \theta_i, \quad \text{for} \quad i \neq r, \quad \theta_r^{(r)} = \theta_r + \alpha_r,$$

then the general operator defined by (10) can be written

$$U_\pm(\theta_\pm, \theta'_\pm) = \prod_{r=0}^{\infty} V_\pm(r; \theta'_r - \theta_r). \tag{11}$$

We note that the simple unitary transformation

$$b(\theta') = e^{i\alpha N}b(\theta)e^{-i\alpha N}$$

is an example of (10) with

$$\theta'_i = \theta_i - 2\alpha.$$

Thus,

$$b(\theta') = e^{-2i\alpha}b(\theta),$$

corresponding to the commutation relation

$$[N, b] = -2b,$$

which is easily checked on a suitable domain. Another simple transformation is

$$b(\theta') = e^{i\alpha N}b(\theta)$$

which gives

$$\theta'_n = \theta_n + n\alpha.$$

We conclude this section by exhibiting some easily verifiable relations valid on obvious domains:

$$\Lambda_\pm = \tfrac{1}{2}(1 \pm e^{i\pi N}),$$
$$[N, b_\pm] = -2b_\pm,$$
$$a^*a = 2b_\pm^*b_\pm + \kappa_\pm,$$
$$a^*a = 2b^*b + \Lambda_-,$$
$$U_\pm^{-1}b_\pm^*b_\pm U_\pm = a^*a,$$
$$U_\pm^{-1}a^*aU_\pm = 2a^*a + \Lambda_-.$$

Note that Eqs. (9) and (3)–(6) give the most general representations of a b and b^* which satisfy $[b, b^*] = 1$, $[N, b] = -2b$, and $\mathfrak{D}_b \supset \mathcal{K}$ = the subspace of $\mathcal{H}$ spanned by finite linear combinations of the states $|n\rangle$.

IV. POWER SERIES REPRESENTATIONS OF b

We want to find an expression for b as a power series in a and a^* on the subspace $\mathcal{K}$. Then the closure of this operator will coincide with the most general b operator of the previous section. We search for all power-series representations on $\mathcal{K}$ of operators b which satisfy the commutation relations

$$[b, b^*] = 1 \tag{12}$$

and

$$[N, b] = -2b. \tag{13}$$

These power series will be found to satisfy Eqs. (3), (5), and (9); again the $b(\theta)$ of the previous section are the only representations of (12) and (13).

Equation (13) holds if and only if b has the form

$$b = \sum_{j=0}^{\infty} \alpha_j a^{*j} a^{j+2}. \tag{14}$$

This expression is well defined on $\mathcal{K}$, since only a finite number of terms will contribute when it operates on any vector in $\mathcal{K}$. We must now determine the α_j so that (14) satisfies (12). We first note that since (14) annihilates both $|0\rangle$ and $|1\rangle$, it must define a reducible representation of (12). Writing

$$b_\pm \equiv b\Lambda_\pm \tag{15}$$

so that

$$b = b_+ + b_-, \tag{16}$$

we see that $b_\pm$ satisfy (12) and (13). Clearly $(b_\pm, \mathcal{H}_\pm)$ are irreducible representations of (12) so that (16) is the irreducible decomposition of b.

It follows from Eq. (14) that

$$b^* |n\rangle = \sum_{k=0}^{n} \bar{\alpha}_k \left[\frac{n!}{(n-k)!} \frac{(n+2)!}{(n-k)!}\right]^{\frac{1}{2}} |n + 2\rangle$$

and

$$b\,|n+2\rangle = \sum_{j=0}^{n} \alpha_j \left[\frac{(n+2)!}{(n-j)!}\frac{n!}{(n-j)!}\right]^{\frac{1}{2}} |n\rangle,$$

so that

$$bb^*\,|n\rangle = F(n)\,|n\rangle \tag{17}$$

and

$$b^*b\,|n\rangle = F(n-2)\,|n\rangle, \quad n \geq 2, \tag{18}$$

where

$$F(n) = n!\,(n+2)!\left|\sum_{j=0}^{n}\frac{\alpha_j}{(n-j)!}\right|^2. \tag{19}$$

Thus Eq. (12) requires that

$$F(n) - F(n-2) = 1, \quad n \geq 2. \tag{20}$$

Furthermore, use of (12) and (17) with $|n\rangle = |0\rangle$, $|1\rangle$ gives

$$F(0) = F(1) = 1. \tag{21}$$

The solution to (20) and (21) is

$$F(2m) = F(2m-1) = m+1, \quad m = 0, 1, 2, \cdots, \tag{22}$$

or

$$F(n) = \tfrac{1}{2}[n + \tfrac{3}{2} + \tfrac{1}{2}(-1)^n]. \tag{23}$$

Now, from Eq. (19) we find that

$$\sum_{j=0}^{n}\frac{\alpha_j}{(n-j)!} = \left[\frac{F(n)}{n!\,(n+2)!}\right]^{\frac{1}{2}} e^{i\theta_n} \equiv R(n), \tag{24}$$

with $\{\theta_n\}$ arbitrary real numbers. Thus,

$$\sum_{j=0}^{n-k}\frac{\alpha_j(-1)^k}{(n-k-j)!\,k!} = \frac{(-1)^k}{k!}R(n-k). \tag{25}$$

We next sum Eq. (25) from $k = 0$ to $k = n$ and interchange the j and k summations to obtain

$$\sum_{j=0}^{n}\sum_{k=0}^{n-j}\frac{\alpha_j(-1)^k}{(n-j-k)!\,k!} = \sum_{k=0}^{n}\frac{(-1)^k}{k!}R(n-k). \tag{26}$$

Using the identities

$$\sum_{k=0}^{r}\frac{(-1)^k}{(r-k)!\,k!} = \begin{cases} 0, & r > 0, \\ 1, & r = 0, \end{cases}$$

Eq. (26) becomes

$$\alpha_n = \sum_{k=0}^{n}\frac{(-1)^k}{k!}R(n-k) = \sum_{j=0}^{n}\frac{(-1)^{n-j}}{(n-j)!}R(j)$$

or, with (23) and (24),

$$\begin{aligned}\alpha_j &= \sum_{r=0}^{j}\frac{(-1)^{j-r}}{(j-r)!}\left[\frac{2r+3+(-1)^r}{4(r!)(r+2)!}\right]^{\frac{1}{2}} e^{i\theta_r} \\ &= \frac{1}{2j!}\sum_{r=0}^{j}\binom{j}{r}(-1)^{j-r}\left[\frac{2r+3+(-1)^r}{(r+2)(r+1)}\right]^{\frac{1}{2}} e^{i\theta_r}. \end{aligned} \tag{27}$$

Thus, Eqs. (12) and (13) require that b have the form (14) with the $\{\alpha_j\}$ given by (27). Conversely, any b having the form (14), (27) will satisfy (12) and (13) on $\mathcal{K}$. We have, therefore, found the most general power-series representation of b on $\mathcal{K}$.

Equations (19) and (23) were deduced above by applying the commutation relation (12) on an n-particle state. An alternate, and instructive, derivation of these equations proceeds as follows. The irreducible components $b_\pm$ of b, defined by Eq. (15), each satisfy (12) and (13):

$$[b_\pm^*, b_\pm] = 1, \tag{28}$$

$$[N, b_\pm] = -2b_\pm. \tag{29}$$

Since the $(b_\pm, \mathcal{K}_\pm)$ are irreducible unitary operators, $U_\pm$ exist satisfying (7) and (8). Multiplication of (29) by $U_\pm^{-1}$ on the left and $U_\pm$ on the right gives

$$[U_\pm^{-1}NU_\pm, a] = -2a,$$

from which one concludes that on $\mathcal{K}$,

$$U_\pm^{-1}NU_\pm = 2N + f_\pm(a) \tag{30}$$

for some functions $f_\pm(a)$ of a only.

Since (30) must be Hermitian, however, the $f_\pm(a)$ must be constants, say $\lambda_\pm$. Finally, application of (30) on the vectors $|\kappa_\pm\rangle$ gives $\lambda_\pm = \kappa_\pm$. Thus we have derived the relation

$$U_\pm^{-1}NU_\pm = 2N + \kappa_\pm, \tag{31}$$

so that

$$N = 2b_\pm^*b_\pm + \kappa_\pm$$

on $\mathcal{K}_\pm$, or

$$N\Lambda_\pm = 2b_\pm^*b_\pm\Lambda_\pm + \kappa_\pm\Lambda_\pm$$

on $\mathcal{K}$. We can also write on $\mathcal{K}$:

$$N = 2b^*b + \Lambda_-. \tag{32}$$

Application of (32) on the state $|n+2\rangle$ now gives the relation

$$n+2 = 2n!\,(n+2)!\left|\sum_{j=0}^{n}\frac{\alpha_j}{(n-j)!}\right|^2 + \tfrac{1}{2}[1-(-1)^n], \tag{33}$$

which is precisely Eqs. (19) and (23). We saw above that (27) is the most general solution to (33).

We have seen that (12) and (13) imply (32). We also see that (13) and (32) determine the most general solution of (12) and (13). Thus, given (13), Eqs. (12) and (32) are equivalent in $\mathcal{K}$.

V. EXPLICIT VERIFICATION THAT THE REPRESENTATIONS OF SECTION IV SATISFY EQUATIONS (3) AND (5)

In Sec. IV we found all the representations of (12) and (13) as power series in a on $\mathcal{K}$. We know, in principle, that any representation of (12) and (13)

must satisfy (3) and (5) with some real numbers $\{\theta_i \mid i = 0, 1, 2, \cdots\}$. We now verify explicitly that this is the case.

We apply the expression (14) for b, with α_j given by (27), on the vector $|n+2\rangle$ to obtain

$$\begin{aligned} b\,|n+2\rangle &= \sum_{j=0}^{n} \alpha_j \frac{[n!\,(n+2)!]^{\frac{1}{2}}}{(n-j)!}\,|n\rangle \\ &= \frac{1}{2}\sum_{j=0}^{n}\sum_{r=0}^{j} \frac{(-1)^{j-r}}{r!\,(j-r)!}\left[\frac{2r+3+(-1)^r}{(r+2)(r+1)}\right]^{\frac{1}{2}} \\ &\quad \times \frac{[n!\,(n+2)!]^{\frac{1}{2}}}{(n-j)!}\, e^{i\theta_r}\,|n\rangle \\ &= \tfrac{1}{2}[n!\,(n+2)!]^{\frac{1}{2}} \sum_{r=0}^{n} \frac{1}{r!}\left[\frac{2r+3+(-1)^r}{(r+2)(r+1)}\right]^{\frac{1}{2}} \\ &\quad \times e^{i\theta_r} \sum_{j=r}^{n} \frac{(-1)^{j-r}}{(j-r)!\,(n-j)!}\,|n\rangle. \end{aligned} \tag{34}$$

Now,

$$\sum_{j=r}^{n} \frac{(-1)^{j-r}}{(j-r)!\,(n-j)!} = \sum_{k=0}^{n-r} \frac{(-1)^k}{k!\,(n-r-k)!} = \delta_{nr},$$

so that (34) becomes

$$b\,|n+2\rangle = \tfrac{1}{2}[2n+3+(-1)^n]^{\frac{1}{2}} e^{i\theta_r}\,|n\rangle, \tag{35}$$

which is precisely equivalent to (3) and (5).

VI. CONSTRUCTION OF THE UNITARY OPERATORS $U_\pm$ RELATING $b_\pm$ AND a

Next we explicitly construct on $\mathcal{K}$ the unitary operators $U_\pm$ defined by Eqs. (7) and (8). It follows from (31) that $U_\pm$ must satisfy

$$U_\pm\,|m\rangle = |2m + \kappa_\pm\rangle e^{i\phi_m^\pm} \tag{36}$$

for some set $\{\phi_j^\pm \mid j = 0, 1, 2, \cdots\}$ of real numbers. We first construct the $U_\pm \equiv U_\pm(\phi_\pm)$ for arbitrary $\{\phi_j^\pm\} \equiv \phi_\pm$ and then determine the specific set $\{\phi_m^\pm\}$ appropriate to the $b^\pm$ defined by $\{\theta_j^\pm\}$.

We can write

$$U_\pm = \sum_{j=0}^{\infty} \beta_j^\pm a^{*2j+\kappa_\pm} a^j P_j, \tag{37}$$

where P_j is the projection operator onto the one-dimensional subspace of $\mathcal{K}$ containing $|j\rangle$. Explicitly

$$P_j = \frac{\sin \pi(N-j)}{\pi(N-j)}.$$

Application of (37) to the vector $|j\rangle$, using (36), gives

$$\beta_j^\pm = \frac{e^{i\phi_j^\pm}}{[j!\,(2j+\kappa_\pm)!]^{\frac{1}{2}}}. \tag{38}$$

The unitarity of the resulting $U_\pm$ on $\mathcal{K}$ can be explicitly verified by applying $U_\pm^\dagger U_\pm$ on the general vector $|n\rangle$.

The above $U_\pm(\phi_\pm)$ will satisfy (31) for any set $\phi_\pm$. To determine the ϕ such that

$$U_\pm^{-1}(\phi_\pm) b_\pm(\theta_\pm) U_\pm(\phi_\pm) = a,$$

we apply the inverted equation

$$U_\pm(\phi_\pm) a U_\pm^{-1}(\phi_\pm) = b_\pm(\theta_\pm)$$

on the general vector $|2m + \kappa_\pm\rangle$ with $m > 0$. We obtain

$$\begin{aligned} (m)^{\frac{1}{2}}\,|2m-2+\kappa_\pm\rangle e^{i(\phi_{m-1}^\pm - \phi_m^\pm)} \\ = (m)^{\frac{1}{2}}\,|2m-2+\kappa_\pm\rangle e^{i\theta_{2m-2+\kappa_\pm}}, \end{aligned}$$

so that we require

$$\phi_m^\pm = \phi_{m-1}^\pm - \theta_{2m-2+\kappa_\pm}, \quad m > 0.$$

Thus,

$$\phi_m^\pm = \phi_0^\pm - \sum_{j=0}^{m-1} \theta_{2j+\kappa_\pm},$$

with $\phi_0^\pm$ arbitrary.

As a special case we explicitly consider the unitary operators $V_\pm(r;\alpha)$ such that

$$V_\pm^{-1}(r;\alpha) b_\pm(\theta_\pm) V_\pm(r;\alpha) = b_\pm(\theta'_\pm),$$

where

$$\theta'_s = \theta_s, \quad \text{for} \quad s \neq r,$$

and

$$\theta'_r = \theta_r + \alpha.$$

From (3) we see that (r even):

$$\begin{aligned} V_+^{-1}(r;\alpha) b_+(\theta_+) V_+(r;\alpha) \\ = \exp\left\{ i\alpha \left[\frac{\sin \pi(N-r-2)}{\pi(N-r-2)}\right]\right\} \cdot b_+(\theta_+). \end{aligned}$$

Assuming that $V_+(r;\alpha)$ is a function of N,

$$V_+(r;\alpha) = V_+(N;r;\alpha),$$

we need only solve

$$V_+^{-1}(N;r;\alpha) V_+(N-2;r;\alpha) = \exp\{\cdots\}. \tag{39}$$

Writing

$$V_+(N;r;\alpha) = e^{iR(N;r;\alpha)},$$

with R Hermitian, (39) becomes

$$R(N-2;r;\alpha) - R(N;r;\alpha) = \alpha \frac{\sin \pi(N-r-2)}{\pi(N-r-2)},$$

which has the solution

$$\begin{aligned} R(N;r;\alpha) \\ = \alpha \frac{|N-r-2| + N - r - 2}{2(N-r-2)} \frac{\sin \pi(N-r)}{\pi(N-r)}. \end{aligned}$$

Thus, $V_+(r;\alpha)$ is given and the general operator $U_+(\theta_+, \theta'_+)$, defined by Eq. (8), is given by Eq. (11). Similar results hold for V_-.

VII. THE IRREDUCIBLE ALGEBRA $\mathcal{A}_+$ OF EVEN POWERS OF a AND a^*

We show that the algebra of operators

$$\mathcal{A}_+ = \left\{\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} c_{ij}(a^*)^{2i}a^{2j}\right\}$$

is irreducible on $\mathcal{H}_+$. Clearly $|0\rangle$ is cyclic in $\mathcal{H}_+$ for the set $\{(a^*)^{2j}, j = 0, 1, 2, \cdots\}$. Now we show that $\mathcal{A}_+$ contains the projection Λ_{+0} onto $|0\rangle$ in $\mathcal{H}_+$. We assert that

$$\Lambda_{+0} = \frac{\sin \pi N_+}{\pi N_+}, \quad N_{+0} \in \mathcal{A}_+,$$

and

$$N_+ |2n\rangle = 2n |2n\rangle. \tag{40}$$

We have $N_+ \in \mathcal{A}_+$ on $\mathcal{K}_+$, the polynomial subspace in $\mathcal{H}_+$, because (40) has the following solution: Let

$$N_+ = \sum_{j=1}^{\infty} c_j(a^*)^{2j}a^{2j}. \tag{41}$$

Then (40) implies

$$\sum_{j=1}^{k} \frac{c_j}{(2k-2j)!} = \frac{1}{(2k-1)!}. \tag{42}$$

Multiply[9] (42) by $\sum_{k=1}^{\infty}(ix)^{2k-1}$ on both sides. Then, after interchanging the order of the j and k summations,

$$\sum_{j=1}^{\infty} c_j \sum_{k=j}^{\infty} \frac{(ix)^{2k-1}}{(2k-2j)!} = \sum_{k=1}^{\infty} \frac{(ix)^{2k-1}}{(2k-1)!}$$

or, recognizing the trigonometric functions,

$$\sum_{j=1}^{\infty} c_j(ix)^{2j-1} \cos x = i \sin x$$

and, after multiplication by $x \sec x$ on both sides and repeated differentiation,

$$c_j = -\frac{(-)^j}{(2j)!}\left(\frac{d}{dx}\right)^{2j}(x \tan x)\Big|_{x=0} \tag{43}$$

or, in terms of Bernoulli numbers,

$$c_j = \frac{(-)^{j+1}2^{2j}(2^{2j}-1)B_{2j-1}}{(2j)!}. \tag{44}$$

By closure, (41) can be assumed to hold in $\mathcal{H}_+$. The relation $N = N_+$ in $\mathcal{H}_+$, i.e., $a^*a = \sum_{j=1}^{\infty} c_j(a^*)^{2j}a^{2j}$ in $\mathcal{H}_+$ implies that $\mathcal{A}_+$ is the algebra generated by a^2 and $(a^*)^2$, since

$$[a^2, (a^*)^2] = 2 + 4a^*a = 2 + 4\sum_{j=1}^{\infty} c_j(a^*)^{2j}a^{2j} \tag{45}$$

in $\mathcal{H}_+$.

To find the power-series representation of b_+ in $\mathcal{K}_+$ in terms of operators in $\mathcal{A}_+$, we use

$$2b_+^*b_+ |2n\rangle = 2n |2n\rangle$$

and

$$b_+ = \sum_{j=0}^{\infty} \beta_j(a^*)^{2j}a^{2j+2}. \tag{46}$$

We find

$$\sum_{j=0}^{n} \frac{\beta_j}{(2n-2j)!} = \frac{e^{i\psi_n}}{[2(2n+1)]^{\frac{1}{2}}} \frac{1}{(2n)!}$$

and, following an argument similar to that just given,

$$\beta_j = \frac{(-)^j}{(2j)!}\left(\frac{\partial}{\partial x}\right)^{2j} \frac{\rho(x)}{\cos x}\Big|_{x=0}, \tag{47}$$

where

$$\rho(x) = \sum_{n=0}^{\infty} \frac{e^{i\psi_n}(ix)^{2n}}{[2(2n+1)]^{\frac{1}{2}}(2n)!}, \tag{48}$$

ψ_n real, arbitrary.

N_- and b_- can be found on their domains in a similar way.

VIII. GENERALIZED BOSE OPERATORS WHICH CREATE AND DESTROY $k\,a$ QUANTA, AND THE LIMIT $k \to \infty$

Results similar to those which we found above for generalized Bose operators $b \equiv b^{(2)}$ satisfying

$$[N, b^{(2)}] = -2b^{(2)}$$

hold for analogous Bose operators satisfying

$$[N, b^{(k)}] = -kb^{(k)}.$$

We sketch the derivation of the coefficients $\alpha_j^{(k)}$ for the Bose operator

$$b^{(k)} = \sum_{j=0}^{\infty} \alpha_j^{(k)} a^{*j}a^{j+k},$$

where

$$[b^{(k)}, b^{(k)*}] = 1. \tag{49}$$

Straightforward calculation shows that

$$bb^* |n\rangle = F(n;k) |n\rangle$$

and

$$b^*b |n\rangle = F(n-k;k) |n\rangle,$$

where

$$F(n;k) = \left| \sum_{j=0}^{n} \frac{[n!\,(n+k)!]^{\frac{1}{2}}}{(n-j)!} \alpha_j^{(k)} \right|^2.$$

Thus, the commutation relation (49) requires

$$F(n;k) - F(n-k;k) = 1, \quad n \geq k,$$

[9] This solution is due to D. I. Fivel (private communication).

and

$$F(n;k) = 1 + [[n/k]],$$

where the symbol $[[x]]$ stands for the greatest integer not exceeding x. Now

$$\sum_{j=0}^{n} \frac{\alpha_j^{(k)}}{(n-j)!} = \left\{\frac{1 + [[n/k]]}{n!\,(n+k)!}\right\}^{\frac{1}{2}} e^{i\theta_n}$$

and use of the binomial identity as before yields

$$\alpha_j^{(k)} = \sum_{l=0}^{j} \frac{(-)^{j-l}}{(j-l)!} \left\{\frac{1 + [[l/k]]}{l!\,(l+k)!}\right\}^{\frac{1}{2}} e^{i\theta_l}.$$

For the remaining discussion, we choose the phases $\theta_n = 0$. We express the integer n as

$$n = sk + \lambda, \quad 0 \leq \lambda < k,$$

where

$$s = [[n/k]], \quad \lambda = n - sk.$$

By direct calculation,

$$\begin{aligned} b^{(k)} |sk+\lambda\rangle &= [F((s-1)k+\lambda;k)]^{\frac{1}{2}} |(s-1)k+\lambda\rangle \\ &= \left\{1 + \left[\left[\frac{(s-1)k+\lambda}{k}\right]\right]\right\}^{\frac{1}{2}} |(s-1)k+\lambda\rangle \\ &= \sqrt{s}\,|(s-1)k+\lambda\rangle, \quad 0 \leq \lambda < k, \end{aligned}$$

and, similarly,

$$b^{(k)*} |sk+\lambda\rangle = (s+1)^{\frac{1}{2}} |(s+1)k+\lambda\rangle, \quad 0 \leq \lambda < k.$$

Also

$$a\,|sk+\lambda\rangle = \begin{cases} (sk+\lambda)^{\frac{1}{2}} |sk+\lambda-1\rangle, & 0<\lambda<k, \\ (sk+\lambda)^{\frac{1}{2}} |(s-1)k+k-1\rangle, & \lambda=0, \end{cases}$$

and

$$a^*\,|sk+\lambda\rangle = \begin{cases} (sk+\lambda+1)^{\frac{1}{2}} |sk+\lambda+1\rangle, & 0 \leq \lambda < k-1, \\ (sk+\lambda+1)^{\frac{1}{2}} |(s+1)k\rangle, & \lambda = k+1. \end{cases}$$

The lower cases of these last two equations represent "edge" effects which we would like to avoid when making a construction to deal with the limit $k \to \infty$. To avoid edges for large k, we define a new decomposition of the integer n:

$$n = (s + \tfrac{1}{2})k + t, \quad -\tfrac{1}{2}k \leq t < \tfrac{1}{2}k,$$

where

$$s = [[n/k]], \quad t = n - (s + \tfrac{1}{2})k,$$

and, to avoid further irrelevant complications, we assume that k is even.

We now construct a larger space $\mathcal{H}_\infty$ in which we can define operators B and B^* which, in a sense to be made precise below, are the limit for $k \to \infty$ of $b^{(k)}$ and $b^{(k)*}$. For each k, the vectors which span the Fock space $\mathcal{H}^{(k)} \equiv \mathcal{H}$ of a and a^* can be labeled by s and t:

$$|s,t\rangle^{(k)} = |(s+\tfrac{1}{2})k + t\rangle, \quad s \geq 0, \quad -\tfrac{1}{2}k \leq t < \tfrac{1}{2}k.$$

An arbitrary vector $\psi^{(k)} \in \mathcal{H}^{(k)}$ has the expansion

$$\psi^{(k)} = \sum_{s\geq 0} \sum_{-\frac{1}{2}k \leq t < \frac{1}{2}k} c_{s,t}^{(k)} |s,t\rangle^{(k)}.$$

Such sequences $\{c_{s,t}^{(k)}\}$ for fixed k form a linear subspace of the Hilbert space $\mathcal{H}_2$ of sequences $\{c_{s,t} \mid s \geq 0, -\infty < t < \infty\}$.

Consider the direct sum

$$\hat{\mathcal{H}} = \bigoplus_{k(\text{even})} \mathcal{H}^{(k)}.$$

An arbitrary vector in $\hat{\mathcal{H}}$ has the form

$$\hat{\Psi} = \bigoplus_k \sum_{s\geq 0} \sum_{-\frac{1}{2}k \leq t < \frac{1}{2}k} c_{s,t}^{(k)} |s,t\rangle^{(k)}.$$

We define $\mathcal{M}$ to be the linear subspace of $\hat{\mathcal{H}}$ for which

$$\lim_{k,l\to\infty} \sum_{s,t} |c_{s,t}^{(k)} - c_{s,t}^{(l)}|^2 = 0,$$

where we take $c_{s,t}^{(k)} = 0$ for s, t outside their allowed ranges. Since $\mathcal{H}_2$ is complete, the $\{c_{s,t}^{(k)}\}$ belonging to a vector in $\mathcal{M}$ converge in $\mathcal{H}_2$ to a sequence $\{c_{s,t}\}$:

$$\lim_{k\to\infty} \sum_{s,t} |c_{s,t}^{(k)} - c_{s,t}|^2 = 0.$$

The vectors in $\mathcal{M}$ can thus be divided into equivalence classes labeled by sequences $\{c_{s,t}\}$ in $\mathcal{H}_2$, and the quotient $\mathcal{H}_\infty = \mathcal{M}/\mathcal{O}$, where $\mathcal{O}$ is the class labeled by the null sequence, is isomorphic to $\mathcal{H}_2$. A complete orthonormal basis in $\mathcal{H}_\infty$ can be labeled by

$$|s,t\rangle = \text{class of } \bigoplus_k |s,t\rangle^{(k)},$$

an arbitrary vector in $\mathcal{H}_\infty$ has the form

$$\Psi = \sum_{s,t} c_{s,t} |s,t\rangle,$$

and the norm in $\mathcal{H}_\infty$ is

$$\|\Psi\|^2 = \sum_{s,t} |c_{s,t}|^2.$$

Note that

$$\|\Psi\| = \lim_{k\to\infty} \|\psi^{(k)}\|$$

for the $\psi^{(k)}$ belonging to any vector in $\mathcal{M}$ in the equivalence class of Ψ.

With this construction, we define operators T and T^* on $\mathcal{M}$[10] as

$$T = \bigoplus_k b^{(k)} \quad \text{and} \quad T^* = \bigoplus_k b^{(k)*}.$$

[10] More precisely, we first define T and T^* on $\mathcal{M} \cap \oplus_k \mathcal{H}^{(k)}$, where $\mathcal{H}^{(k)} \equiv \mathcal{H}$, and then extend them by closure. All of the operators defined in this section should be understood in this sense.

In particular,

$$T \bigoplus_k |s, t\rangle^{(k)} = \bigoplus_k (s)^{\frac{1}{2}} |s-1, t\rangle^{(k)}$$

and

$$T^* \bigoplus_k |s, t\rangle^{(k)} = \bigoplus_k (s+1)^{\frac{1}{2}} |s+1, t\rangle^{(k)}.$$

Since T and T^* leave $\mathcal{O} \cap \bigoplus_k \mathcal{K}$ invariant, they induce operators B and B^* on $\mathcal{H}_\infty$, which can be taken as the "limits" of $b^{(k)}$ and $b^{(k)*}$ for $k \to \infty$. We have

$$B |s, t\rangle = (s)^{\frac{1}{2}} |s-1, t\rangle$$

and

$$B^* |s, t\rangle = (s+1)^{\frac{1}{2}} |s+1, t\rangle.$$

Note that

$$\langle s', t'| B |s, t\rangle = \lim_{k\to\infty} {}^{(k)}\langle s', t'| b^{(k)} |s, t\rangle^{(k)}.$$

We also define limits constructed from a and a^*. Let $a^{(k)}$ and $a^{(k)*}$ act on $\mathcal{H}^{(k)}$ via

$$a^{(k)} |s, t\rangle^{(k)} = [(s+\tfrac{1}{2})k + t]^{\frac{1}{2}} |s, t-1\rangle^{(k)}$$

and

$$a^{(k)*} |s, t\rangle^{(k)} = [(s+\tfrac{1}{2})k + t + 1]^{\frac{1}{2}} |s, t+1\rangle^{(k)}.$$

Because $\|a^{(k)} |s, t\rangle^{(k)}\|$ and $\|a^{(k)*} |s, t\rangle^{(k)}\|$ grow with k, $\bigoplus_k a^{(k)}$ and $\bigoplus_k a^{(k)*}$ do not exist in $\mathcal{M}$. However,

$$\bigoplus_k (a^{(k)}/k^{\frac{1}{2}}) |s, t\rangle^{(k)} = \bigoplus_k [(s+\tfrac{1}{2}) + tk^{-1}]^{\frac{1}{2}} |s, t-1\rangle^{(k)}$$
$$\sim (s+\tfrac{1}{2})^{\frac{1}{2}} \bigoplus_k |s, t-1\rangle^{(k)}$$

(where $\sim$ indicates the above equivalence) and, similarly,

$$\bigoplus_k (a^{(k)*}/k^{\frac{1}{2}}) |s, t\rangle^{(k)} \sim (s+\tfrac{1}{2})^{\frac{1}{2}} \bigoplus_k |s, t+1\rangle^{(k)}.$$

The operators

$$\bigoplus_k (a^{(k)}/k^{\frac{1}{2}}) \quad \text{and} \quad \bigoplus_k (a^{(k)*}/k^{\frac{1}{2}})$$

in $\mathcal{M}$[10] induce operators A_0 and A_0^* in $\mathcal{H}_\infty$:

$$A_0 |s, t\rangle = (s+\tfrac{1}{2})^{\frac{1}{2}} |s, t-1\rangle$$

and

$$A_0 |s, t\rangle = (s+\tfrac{1}{2})^{\frac{1}{2}} |s, t+1\rangle.$$

In a similar way, the operators

$$\bigoplus_k 2k[(a^{(k)}/k^{\frac{1}{2}}) - (s+\tfrac{1}{2})^{\frac{1}{2}} c_-^{(k)}]$$

and

$$\bigoplus_k 2k[(a^{(k)*}/k^{\frac{1}{2}}) - (s+\tfrac{1}{2})^{\frac{1}{2}} c_+^{(k)}],$$

where

$$c_\pm^{(k)} |s, t\rangle^{(k)} = |s, t \pm 1\rangle^{(k)},$$

in $\mathcal{M}$ induce operators A_1 and A_1^* in $\mathcal{H}_\infty$:

$$A_1 |s, t\rangle = \frac{t}{(s+\frac{1}{2})^{\frac{1}{2}}} |s, t-1\rangle$$

and

$$A_1^* |s, t\rangle = \frac{t+1}{(s+\frac{1}{2})^{\frac{1}{2}}} |s, t+1\rangle.$$

More generally, the operators

$$\bigoplus_k \frac{n!\, k^n}{\frac{1}{2}(-\frac{1}{2})\cdots(\frac{3}{2}-n)} \times \left[\frac{a^{(k)}}{k^{\frac{1}{2}}} - \sum_{j=0}^{n-1} \frac{(\frac{1}{2})(-\frac{1}{2})\cdots(\frac{3}{2}-j)}{j!\,(s+\frac{1}{2})^{j-\frac{1}{2}}} \left(\frac{t}{k}\right)^j c_\mp^{(k)}\right]$$

in $\mathcal{M}$ induce operators A_n and A_n^* in $\mathcal{H}_\infty$:

$$A_n |s, t\rangle = \frac{t^n}{(s+\frac{1}{2})^{n-\frac{1}{2}}} |s, t-1\rangle$$

and

$$A_n^* |s, t\rangle = \frac{(t+1)^n}{(s+\frac{1}{2})^{n-\frac{1}{2}}} |s, t+1\rangle.$$

The commutation relations among these operators can be found straightforwardly. For example, of course,

$$[B, B^*] = 1.$$

Some other commutators are

$$[A_0, A_0^*] = 0, \quad [A_1, A_1^*] = \frac{2t+1}{s+\frac{1}{2}},$$

$$[A_n, A_n^*] = \frac{(t+1)^{2n} - t^{2n}}{(s+\frac{1}{2})^{2n-1}},$$

$$[B, A_0] |s, t\rangle = (s)^{\frac{1}{2}}[(s+\tfrac{1}{2})^{\frac{1}{2}} - (s-\tfrac{1}{2})^{\frac{1}{2}}] |s-1, t-1\rangle.$$

The operators

$$B^*B |s, t\rangle = s |s, t\rangle$$

and

$$\tfrac{1}{2}(A_0^*A_1 + A_1^*A_0) |s, t\rangle = t |s, t\rangle$$

are Hermitian number operators. Finally, we remark that $|0, t\rangle$ are no-particle vectors for B and $|0, t\rangle$ are cyclic for polynomials in B^*, A_0, and A_0^*.

This construction produces a Hilbert space $\mathcal{H}_\infty$ in which, heuristically speaking, operators B and B^* annihilating and creating infinite numbers of a quanta exist together with operators A_n and A_n^* which annihilate and create single a quanta. A construction of this kind might be of use in the description of a quantized hydrodynamic system with finite average density and infinite volume, where operators analogous to B and B^* would change the average density and operators analogous to A_n and A_n^* would produce local changes in density.

IX. CONCLUDING REMARKS

We can consider the power-series representations of the generalized Bose operators b to be generated by imposing Bose commutation relations on an operator which is equivalent to two a quanta. The leading term $b \sim \alpha_0 a^2$ gives a commutator which is not a c-number, and the remaining terms of the infinite series are necessary to remove the operator terms from the commutator. For applications, the first coefficient α_0 which expresses the relation between the state $b^* |0\rangle$ of one b operator and the state $a^{*2} |0\rangle$ of two a operators would be most important. The higher coefficients give relations such as

$$b^* a^* |0\rangle = (\bar{\alpha}_0 + \bar{\alpha}_1) a^{*3} |0\rangle$$

and, in a more realistic situation, would contain information about the interaction between a and b quanta, and thus would also be of interest.

We plan to explore, in the context of a relativistic four-dimensional situation, the possibility that an unstable particle or resonant state can be described by a generalized free field. Assuming asymptotic irreducibility (or via Ruelle's Theorem,[11] just asymptotic completeness), this generalized free field should exist in the Hilbert space of the in (or out) fields of the stable particles of the theory and, indeed, Streit's analysis, extended straightforwardly to include internal degrees of freedom, guarantees this existence. The leading terms in the power-series representation of the creation part of a generalized free field representing an unstable particle will contain the creation parts of the out fields of the stable decay products together with a c-number coefficient which is the decay amplitude for the relevant decay mode. The condition that the field of the unstable particle be a generalized free field, together with kinematical constraints, leads to exact relations among the decay amplitudes and a small number of amplitudes for the inelastic scattering of the unstable particle by its decay products, provided the decay products have nonzero mass. For massless decay particles, similar approximate relations can be found based on the smallness of the amplitudes for emission of several massless particles. We expect that approximate relations between the inelastic scattering amplitudes and the decay amplitudes can be found, and that, based on these relations, we will be able to test experimentally the hypothesis that unstable particles can be described by a generalized free field.

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ACKNOWLEDGMENTS

We thank Professor E. J. Woods for many useful suggestions and for a careful reading of the manuscript, Professor D. I. Fivel for the solution to Eq. (42), and Professor A. J. Dragt and Professor J. M. Horvath for helpful discussions.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

Existence of Solutions for Certain Nonlinear Boundary-Value Problems*

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(Received 25 November 1968)

The existence of solutions of a class of nonlinear boundary-value problems is characterized in terms of a linear eigenvalue problem. Bounds and comparison results for solutions are derived.

1. INTRODUCTION

Several recent papers[1-3] have studied nonlinear boundary-value problems of the form

$$y''(x) + r^2(x)y(x) - y^n(x) = 0, \tag{1}$$

$$y(0) = 0 = y(\pi) \tag{2}$$

which have arisen in connection with the distribution of energy in a nuclear power reactor. The exponent $n \geq 2$ is not necessarily an integer. For simplicity we discuss problems with continuous $r^2(x)$ though for the most part piecewise continuity would suffice.

On physical grounds it has been conjectured that there is a unique positive solution of (1) and (2). Keller has shown[3] that, if there is a positive solution, it is unique. We shall prove that *a positive solution exists if and only if the largest eigenvalue of* (2) *and*

$$y''(x) + r^2(x)y(x) = \lambda y(x) \tag{3}$$

is positive. Our constructive approach does yield a feasible computational procedure, but we are mainly concerned with this characterization and some useful implications of our proof.

2. EXISTENCE

We shall need Keller's result that, if there is a positive solution $y(x)$ of (1) and (2), then it is unique. A simple argument[3] also gives the bound

$$0 \leq y(x) < R^{1/(n-1)}, \tag{4}$$

where R is the maximum value of $r^2(x)$. Let us correspondingly define ρ as the minimum value of $r^2(x)$.

Let $\lambda_1, y_1(x)$ be the largest eigenvalue and associated eigenfunction of (2) and (3). Because $r^2(x) \in C[0, \pi]$ it is known[4] that $y_1(x) \in C^2[0, \pi]$ and $y_1(x) > 0$ for $0 < x < \pi$. Suppose now (1) and (2) have a positive solution $y(x) \in C^2[0, \pi]$. Multiply (1) by $y_1(x)$ and (3) by $y(x)$, then subtract the resulting equations. Integrating the difference over $[0, \pi]$ and using the boundary conditions (2), we are led to

$$\lambda_1 \int_0^\pi y_1(x)y(x)\,dx = \int_0^\pi y_1(x)y^n(x)\,dx.$$

Both integrals are obviously positive, which implies $\lambda_1 > 0$. This shows that for a positive solution to exist it is necessary that λ_1 be positive.

Existence and some other useful results will be demonstrated by a general method. We can rewrite (1) as $-y''(x) + a(x)y(x) = [r^2(x) + a(x)]y(x) - y^n(x)$ and accordingly define

$$Ly(x) = -y''(x) + a(x)y(x),$$
$$F(x, y) = [r^2(x) + a(x)]y - y^n.$$

To apply the method we must find curves $u(x)$, $U(x)$ such that

$$\begin{aligned} u(x) &\leq U(x), \quad \text{for all } x, \\ u(0) &\leq 0, \quad u(\pi) \leq 0, \\ U(0) &\geq 0, \quad U(\pi) \geq 0, \\ LU(x) &\geq F(x, U(x)), \\ Lu(x) &\leq F(x, u(x)), \end{aligned} \tag{5}$$

and we must choose $a(x) \geq 0$ such that $F(x, y)$ is a monotonic increasing function of y for all (x, y) in the set

$$S = \{(x, y) \mid 0 \leq x \leq \pi, u(x) \leq y \leq U(x)\}.$$

It then follows[5] that (1) and (2) have at least one solution that lies entirely in S; there is a largest solution $w(x)$ in S, meaning that if $y(x)$ is a solution of (1) and (2) in S, then

$$y(x) \leq w(x), \quad \text{for} \quad 0 \leq x \leq \pi,$$

and the sequence $\{v_k(x)\}$, defined by $v_0(x) = U(x)$,

$$Lv_k(x) = F(x, v_{k-1}(x)), \quad v(0) = 0 = v(\pi),$$

converges monotonically and uniformly downwards to $w(x)$:

$$w(x) \leq \cdots \leq v_k(x) \leq \cdots \leq v_0(x), \quad \text{for } 0 \leq x \leq \pi.$$

First we wish to observe that if there is a positive solution it can always be constructed in this way. To see this we note that the trivial solution $u(x) = 0$

* This work was supported by NSF Grant 5967.

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satisfies the requirements on u. We know that a positive solution must satisfy (4) so let us try

$$U(x) \equiv R^{1/(n-1)}.$$

Now

$$\frac{\partial F}{\partial y} = r^2(x) + a(x) - ny^{n-1} \geq 0, \quad \text{on } S,$$

if we only require

$$a(x) \geq nR - \rho > 0.$$

Since

$$LU(x) - F(x, U(x)) = R^{1/(n-1)}[R - r^2(x)] \geq 0,$$

all the requirements are satisfied. By (4) any positive solution lies in S and the general method says it is the limit of the $\{v_k(x)\}$.

At this point we still do not know if there is a nontrivial solution of (1) and (2). This will follow, though, if we can find a $u(x)$ such that $u(x) \geq 0$ and $u(x) \not\equiv 0$, since the solution in S satisfies $y(x) \geq u(x)$ and, hence, cannot be trivial. Pursuing this line of thought, we can obtain a useful comparison result. Suppose that for some $r_1^2(x)$ the problem (1), (2) has a positive solution $u(x)$ and we are interested in the problem with $r_2^2(x) \geq r_1^2(x)$ for all x. Then

$$\begin{aligned} Lu(x) &= [r_1^2(x) + a(x)]u(x) - u^n(x) \\ &\leq [r_2^2(x) + a(x)]u(x) - u^n(x) = F(x, u(x)). \end{aligned}$$

By (4), $u(x) \leq U(x)$ and all the other conditions are obvious. Thus it follows that this problem has a positive solution $y(x)$ and moreover $y(x) \geq u(x)$; that is, increasing $r^2(x)$ increases the positive solution.

To complete the existence discussion suppose the eigenvalue λ_1 of (2) and (3) is positive. Normalize the eigenfunction such that

$$\lambda_1 \geq y_1^{n-1}(x) \quad \text{and} \quad R \geq y_1^{n-1}(x). \tag{6}$$

We claim that we can take $u(x) = y_1(x)$. The latter normalization condition states $U(x) \geq u(x)$ and the former implies

$$\begin{aligned} Lu(x) &= [r^2(x) + a(x)]u(x) - \lambda_1 u(x) \\ &\leq [r^2(x) + a(x)]u(x) - u^n(x) = F(x, u(x)). \end{aligned}$$

Thus, existence of a positive solution and a nontrivial lower bound follow in the usual way.

3. EXAMPLES AND APPLICATIONS

The sequence $\{v_k(x)\}$, which decreases to the positive solution, can be used as a computational procedure on calculating $v_k(x)$ with a method for linear problems, e.g., finite differences. This is likely to be pretty satisfactory until the average value of $r^2(x)$ becomes large and it becomes necessary to use singular perturbation methods to handle the boundary layer.[3] If a careful choice of $a(x)$ is made, it may be possible for specific problems to compute analytical bounds. We shall now develop an upper bound better than (4) for all problems.

Let us use the constant $a = nR - \rho$ and define $z(x)$ as the solution of

$$Lz(x) = 0, \quad z(0) = R^{1/(n-1)} = z(\pi),$$

$$z(x) = R^{1/(n-1)} \frac{\cosh (nR - \rho)^{\frac{1}{2}}(x - \frac{1}{2}\pi)}{\cosh (nR - \rho)^{\frac{1}{2}}\frac{1}{2}\pi}.$$

Consider $U(x) = R^{1/(n-1)} - z(x)$. Obviously, $z(x) > 0$, so if we use the monotonicity of $F(x, y)$,

$$\begin{aligned} F(x, U(x)) - LU(x) &\leq F(x, R^{1/(n-1)}) - aR^{1/(n-1)} \\ &= R^{1/(n-1)}[r^2(x) - R] \leq 0. \end{aligned}$$

Thus, (5) holds for this $U(x)$ and clearly $U(0) = 0 = U(\pi)$. To see that $U(x)$ is an upper bound for a positive solution which we suppose exists, let us normalize $y_1(x)$ such that (6) holds and

$$U(x) \geq y_1(x) = u(x)$$

which can certainly be done. Then the existence theorem asserts that

$$y(x) \leq R^{1/(n-1)} - z(x). \tag{7}$$

Other authors[3] have studied the case when $r(x)$ is a constant μ. The eigenvalue problem (2), (3) has $\lambda_1 = \mu^2 - 1$ so there is a positive solution of (1) and (2) if and only if $\mu > 1$.

Since $R = \mu^2$, the eigenfunction normalized as in (6) is

$$y_1(x) = (\mu^2 - 1)^{1/(n-1)} \sin x.$$

This is not only a lower bound for the special case $r^2(x) = \mu^2$ but, using our comparison result, is also a lower bound for the positive solution for any $r^2(x) \geq \rho = \mu^2 > 1$. Thus (7) with this $y_1(x)$ gives improved upper and lower bounds for all such problems:

$$(\rho - 1)^{1/(n-1)} \sin x \leq y(x) \leq R^{1/(n-1)} - z(x).$$

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

Algorithm for the Calculation of the Classical Equations of Motion of an N-Body System*

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(Received 25 March 1968)

The equations of motion for N-body systems are usually integrated by means of a *central-difference* algorithm. An alternative *average force* algorithm is described in this paper. The new method is shown to have both theoretical and practical advantages when compared to the central-difference method.

INTRODUCTION

This algorithm was developed to facilitate our computer simulation investigations of various radiation-damage phenomena. It has been thoroughly tested in situations where most of the interacting particles are initially arranged into an ordered lattice structure. As the simulation progresses, this ordering rapidly decays, so we have every reason to believe that it would be equally effective in situations where the N bodies are originally randomly distributed. The algorithm has been tested in systems where $\sim 25 \leq N \leq \sim 500$. Cost considerations, program running time, and available memory size are the only apparent limitations on N.

The original Brookhaven National Laboratory investigation of radiation-damage events by computer simulation[1] has remained the only complete discussion of the criteria which must be satisfied before the simulation method can be applied. Their calculations utilize the familiar central-difference (CD) method of integration. Here, we discuss an alternative integration procedure, the average force (AF) method, but always within the criteria established in the Brookhaven paper. This algorithm has been mentioned in the literature,[2] but a detailed presentation of its rationale and implications has never been made.

I. THE PROBLEM

Consider a system of N interacting bodies which move subject to the laws of Newtonian mechanics. We assume that the force on the αth member of the set $\mathbf{F}_\alpha$ is a function of the positions of *all* of the bodies in the system $\mathbf{F}_\alpha = \mathbf{F}_\alpha(\mathbf{r}_1, \cdots, \mathbf{r}_n)$. We further assume that this force can be expressed as the sum of pairwise interactions between the αth body and all of the other members of the set:

$$\mathbf{F}_\alpha = \sum_{n \neq \alpha}^{N} \mathbf{F}_{\alpha n}(\mathbf{r}_{\alpha n}),$$

$$\mathbf{r}_{\alpha n} \equiv \mathbf{r}_\alpha - \mathbf{r}_n .$$

Although the αth body moves under the influence of $\mathbf{F}_\alpha$,

$$\mathbf{F} = m_\alpha \ddot{\mathbf{r}}_\alpha ,$$

it will be sufficient for our purposes to examine an equivalent one-dimensional problem in which we investigate the motion of m_α under the influence of one component, the ith, of one of the $\mathbf{F}_{\alpha n}$. It will be convenient to assume that this force component $F_{i\alpha}$ is the strongest force component which m is experiencing at that time. The other force components exist, but we shall include their effect later. We temporarily suppress all indices except i, and write

$$m\dot{v}_i(t) = F_i[x_i(t), v_i(t)]. \tag{1}$$

To simplify the notation we have not indicated the explicit dependence of F_i upon the positions of all of the other bodies in the system, but this dependence is always present. As usual,

$$\dot{v}_i(t) = dv_i(t)/dt \tag{2}$$

and

$$\dot{x}_i(t) = v_i(t) = dx_i(t)/dt. \tag{3}$$

We wish to study the numerical integration of Eqs. (1)–(3) by finite-difference methods. The integration process will be subject to three criteria:

(1) We require a minimum number of computations per time increment Δt;

(2) we require a minimum number of time increments to accomplish a particular displacement; and

(3) we shall use the *energy decrement*

$$\Delta E = |[E(t') - E(t)]/E(t)|,$$

where

$$E(t) = \tfrac{1}{2}mv_i^2(t) + U[x_i(t), v_i(t)],$$

and $U[x_i(t), v_i(t)]$ is the body's potential energy, as a measure of excellence for the integration process.

* This work was supported by the Office of Naval Research.

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II. THE CENTRAL-DIFFERENCE METHOD

In finite-difference form, Eqs. (1)–(3) become, when (1) and (2) are combined,

$$m^{-1}F_i[x_i(t)] \cong [v_i(t + \Delta t/2) - v_i(t - \Delta t/2)]/\Delta t, \quad (4)$$

$$v_i(t + \Delta t/2) \equiv \dot{x}_i(t + \Delta t/2) \cong [x_i(t + \Delta t) - x_i(t)]/\Delta t. \quad (5)$$

Equation (4) can be immediately rearranged to read

$$v_i(t + \Delta t/2) \simeq v_i(t - \Delta t/2) + F_i[x_i(t)]m^{-1}\Delta t, \quad (6)$$

while, after rearrangement and substitution from Eq. (6), Eq. (5) becomes

$$x_i(t + \Delta t) \simeq x_i(t) + v_i(t - \Delta t/2)\Delta t + F_i[x_i(t)]m^{-1}\Delta t^2. \quad (7)$$

When initial values $v_{i0} = v_i(t_0 - \Delta t/2)$ and $x_{i0} = x_i(t_0)$ and a *timestep* Δt have been established, Eqs. (6) and (7) comprise a consistent self-regenerating set.

From a practical point of view, this integration algorithm is inconvenient if we wish to go beyond the basic determination of $x_i(t)$ and consider other physical quantities, because it does not give simultaneous determinations of position and velocity. Momentum conservation can be built into the N-body system, but determination of the total energy $E(t)$ is complicated by this property of the method.

This algorithm is based upon the tacit assumption that $v_i(t + \Delta t/2)$ is in some sense the mean of $v_i(t)$ and $v_i(t + \Delta t)$, so the "average" velocity is used in calculating the displacement $\Delta x_i = x_i(t + \Delta t) - x_i(t)$. Similarly, the force determined at time t, $F[x_i(t)]$, is the "average" force between $x_i(t - \Delta t/2)$ and $x_i(t + \Delta t/2)$ which is required to determine the change in velocity. The AF algorithm described in the next section is mathematically less rigorously justified than the CD algorithm, but it is designed to exploit the "average" nature of the various quantities required in the integration in ways which overcome the practical difficulties of the CD method.

III. THE AVERAGE-FORCE METHOD

In the discussion of the AF method we use a timestep ΔT. Thus, formulas which contain Δt are CD formulas, while AF results depend upon ΔT. Later we shall show that Δt and ΔT can be mathematically related by direct application of the criteria of excellence presented above.

The AF algorithm is based upon the Taylor's series expansion of $x_i(t + \Delta T)$ about $x_i(t)$. This expansion gives

$$x_i(t + \Delta T) = x_i(t) + v_i(t)\Delta T + a_i(t)\Delta T^2/2 + a_i(t)\Delta T^3/6 + \cdots.$$

In a constant-force problem, all coefficients of ΔT^n, with $n \gg 2$, vanish; so we *define* Δv_i such that

$$x_i(t + \Delta T) = x_i(t) + v_i(t)\Delta T + \Delta v_i \Delta T/2.$$

With this definition, Δv_i is the average charge in velocity during the internal ΔT. We now use Δv_i to introduce an average force $\langle F_i \rangle$:

$$\Delta v_i \equiv \langle F_i \rangle m^{-1}\Delta T. \quad (8)$$

Then,

$$v_i(t + \Delta T) = v_i(t) + \langle F_i \rangle m^{-1}\Delta T \quad (9)$$

and

$$x_i(t + \Delta T) = x_i(t) + [v_i(t) + \langle F_i \rangle \Delta T/2m]\Delta T \quad (10)$$

are the AF equivalents of Eqs. (6) and (7).

We obtain two advantages by this trivial modification of the CD method:

(1) the position and velocity are determined simultaneously, and

(2) physical intuition can be used to develop approximate values for $\langle F_i \rangle$ which will improve the precision of the numerical integration process.

The major conceptual difference between the CD and AF methods can be summarized as follows: In the CD method, the force is exactly known but the equations [Eqs. (6) and (7)] are only asymptotically correct, while in the AF method the equations [Eq. (9) and (10)] are exact, but the average force must be determined by an ancilliary argument.

Equations (7) and (10) can be converted into mathematically identical forms. To see this we make a Taylor's series expansion of $v_i(t - \Delta t/2)$ and retain only two terms:

$$v_i(t - \Delta t/2) \doteq v_i(t) - (\Delta t/2)\dot{v}_i(t).$$

When this result is used in Eq. (7), together with Eq. (1), to eliminate $\dot{v}_i$, we obtain

$$x_i(t + \Delta t) = x_i(t) + \Delta t\{v_i(t) + F_i[x_i(t)]\Delta t/2m\}. \quad (11)$$

Equations (10) and (11) are formally equivalent, except that $\langle F_i \rangle$ and $F_i[x_i(t)]$ must be interpreted differently. This formal similarity first led us to explore the AF method.

IV. DETERMINATION OF $\langle F_i \rangle$

For the moment, presume that the function $F_i[x_i(t)]/m$ is known exactly. Figure 1 shows four possible graphs of $F_i[x_i(t)]/m$ vs $x_i(t)$. In each case, the area under the curve is Δv_i, while the area enclosed by the broken-line rectangle is the Δv_i obtained by a CD computation. In this section, we presume that Δv_i is "small" compared to $v_i(t)$, but will defer a definition of "small" to a later section.

Let us rewrite Eq. (10) in the form

$$\Delta x_i \equiv x_i(t + \Delta T) - x_i(t) = v_i(t)\Delta T + \Delta v_i \Delta T/2,$$

and look at one of the sections of Fig. 1 in more detail. In Fig. 2, the line labeled x_i' indicates the value of Δx_i obtained when Δv_i is neglected. We note that this position is completely independent of $F_i(t)/m$. Further, we note that if Δv_i is "small" compared to v_i, the difference $x_i(t + \Delta t) - x_i'$ will always be "small" compared to Δx_i.

It is convenient to think of each timestep as a two-stage process:

(1) Move the body to $x_i'(t + \Delta T)$, the new position produced by

$$x_i'(x + \Delta T) \equiv x_i(t) + v_i(t)\Delta T,$$

(2) Compute the additional displacement $\Delta v_i \Delta T/2$ as accurately as possible. Because the force functions used in this type of calculations is not pathological, we may presume that $F[x'(t + \Delta T)]$ is a better approximation to $F[x(t + \Delta T)]$ than is $F[x(t)]$. Thus, if we define a first approximation to Δv_i by $\Delta v_i^{(1)} = F[x(t)]\Delta T/m$, it seems reasonable that

$$\Delta v_i^{(2)} = \{F[x'(t + \Delta T)] + F[x(t)]\}\Delta T/2m$$

is a better approximation to Δv_i. This, of course, presumes that ΔT is chosen sufficiently small that a trapezoid-rule integration of the force to obtain Δv_i is a reasonable approximation.

This series of approximations can conveniently be carried one step further. We define

$$x_i^*(t + \Delta T) = x_i(t) + v_i(t)\Delta T + F_i[x_i(t)]\Delta T^2/2m, \tag{12}$$

which is the location the body would reach if F_i remained constant for the period ΔT. We note that $x_i^*(t + \Delta T) = x_i(t + \Delta t)$, the CD result calculated

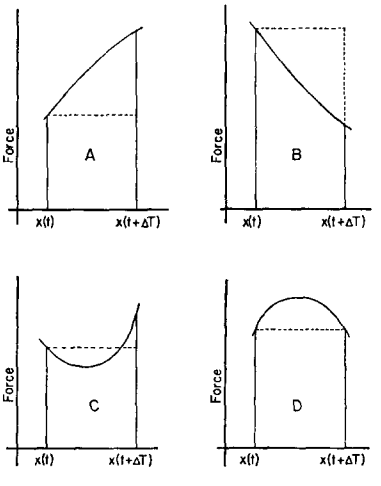

FIG. 1. The force can change in various ways in the course of a single timestep. Here the actual force is compared with the force used in a CD calculation (broken line) for four possible cases.

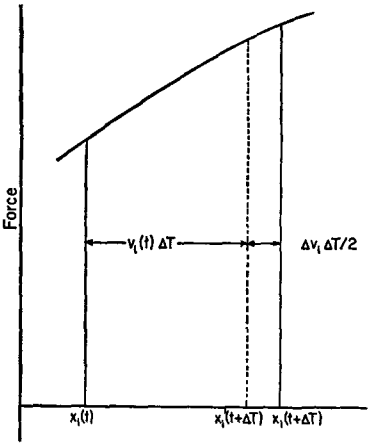

FIG. 2. Most of the displacement in a single timestep is the result of the velocity which exists at the beginning of that timestep ($v_i(t)\Delta T$). Thus $F_i[x'(t + \Delta T)]$ is a good first approximation to

$F_i[x(t + \Delta T)]$.

with $v_i = v_i(t)$ instead of $v_i(t - \Delta t/2)$. Thus,

$$x_i^*(t + \Delta T)$$

is effectively equivalent to the position at the end of the timestep as computed by the CD method. In terms of this position, we define a third approximation to Δv_i by writing

$$\Delta v_i^{(3)} = \{F_i[x_i^*(t + \Delta T)] + F_i[x_i(t)]\}\Delta T/2m. \tag{13}$$

This is equivalent to defining

$$\langle F_i \rangle \equiv \tfrac{1}{2}\{F_i[x_i^*(t + \Delta T)] + F_i[x_i(t)]\}. \tag{14}$$

The steps of the AF method may be summarized as follows:

(1) make a preliminary calculation of the new position using Eq. (12);

(2) determine the force at that position;

(3) average the force calculated in step 2 with $F_i[x_i(t)]$; and

(4) use the average force calculated in step 3 to compute $v_i(t + \Delta T)$ and $x_i(t + \Delta T)$ from Eqs. (9) and (10).

It is immediately apparent that the AF method will make an improvement in v_i calculation for cases a and b in Fig. 1, and it will be no less accurate than the CD method in cases c and d. However, it appears to be much slower to implement on the computer because a single AF timestep requires almost as many computations as two CD timesteps. We shall now show that, although additional calculations are required per timestep, the AF method requires fewer timesteps for a given total displacement with a smaller energy decrement.

V. DETERMINATION OF ΔT

A. Comparison of ΔT and Δt

We use the following criterion to establish a relationship between Δt and ΔT, the timestep in the two methods:

A timestep must terminate when the difference between the force at its end and the force used in the integration equals or exceeds a preset value.

For the moment we do not attempt to establish the value of this difference, but we do require that the same value apply to each method. Then we can write

$$F_i[x(t+\Delta t)] - F_i[x(t)] = F_i[x(t+\Delta T)] - \langle F_i\rangle. \tag{15}$$

If we now substitute the definition of $\langle F_i\rangle$, Eq. (14), into Eq. (15) and expand

$$F_i[x_i(t+\Delta t)],$$
$$F_i[x_i(t+\Delta T)],$$

and

$$F_i[x_i^*(t+\Delta T)]$$

in Taylor's series, after some algebra, we obtain

$$[x_i(t+\Delta t) - x_i(t)]\left(\frac{dF_i}{dx_i}\right)_t = [x_i(t+\Delta T) - x_i(t)]\left(\frac{dF_i}{dx_i}\right)_t - \tfrac{1}{2}[x_i^*(t+\Delta T) - x_i(t)]\left(\frac{dF_i}{dx_i}\right)_t, \tag{16}$$

which is correct to terms of the order of x_i. To this same approximation, we find that

$$x_i(t+\Delta t) - x_i(t) = v_i(t - \Delta t/2)\Delta t,$$
$$x_i(t-\Delta T) - x_i(t) = v_i(t)\Delta T,$$

and

$$x_i^*(t-\Delta T) - x_i(t) = v_i(t)\Delta T.$$

When these results are substituted into Eq. (16), we obtain

$$v_i(t - \Delta t/2)\Delta t = v_i(t)\Delta T/2. \tag{17}$$

But we have already assumed that v_i does not make a large change in one timestep, so, approximately, $\Delta T \doteq 2\Delta t$. We expect that the AF method will tolerate a timestep, which is twice the CD timestep, and still produce roughly equivalent accuracy. This property of the AF method has been extensively tested over a broad energy range, 0.001 eV to 10 keV, and has always been found to hold true.

Actually, when $\Delta T = 2\Delta t$, we find that AF method gives a considerably smaller energy decrement in ~90% of the cases tested and never gives a large decrement. We can justify this property graphically. Figure 3 shows the work done, as calculated by each method, in two cases. In case a, we see that the CD method under-estimates the work by an amount $A = A_1 + A_2$; in case b, it over-estimates the work by an amount $B = A_1 + A_2$. In both of these cases

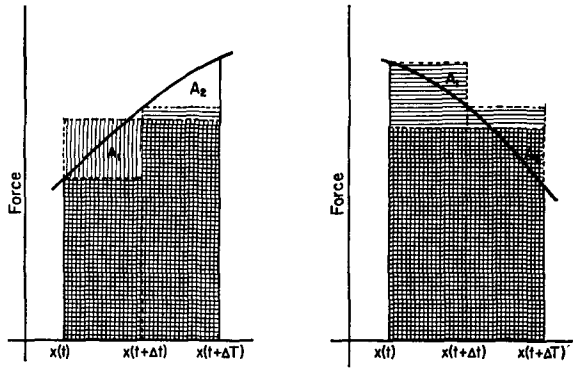

FIG. 3. The vertical hatching is the work as approximated by the AF method, the horizontal by the CD method. The curvature in the force curve is somewhat larger than we might expect in a normal timestep. In both cases the AF method gives a better approximation to the work done during the timestep (the area under the curve) than does the CD method.

the AF calculation gives almost exactly the correct amount of work, because F is changing almost linearly with x. In cases c and d, the AF calculation is also in error by roughly the same amount as the CD calculation and, in extreme cases, it is actually possible for the CD calculation to be more accurate. In actual operation cases a or b occur ~90% of the time, so the AF method almost always gives better results than the CD method when the computation is extended over a number of timesteps. Identical test situations run over 100 AF timesteps (200 CD timesteps) show that the energy decrement is noticably smaller in the AF than in the CD calculation. To make quantitative comparisons between the two methods we must examine the relationship between the energy decrement and the timestep length.

B. Choice of ΔT

It is convenient to define ΔT in terms of the maximum displacement component of the most energetic body in the system. We first rewrite Eq. (10) in the form

$$\Delta x_i = (v_i + \langle F_i\rangle\Delta T/2m)\Delta T,$$

so that

$$\Delta T = \Delta x_i/(v_i + \langle F_i\rangle\Delta T/2m). \tag{18}$$

In normal applications $v_i \gg \langle F_i\rangle\Delta T/2m$, or the computation is not accurate, so we may approximate

$$\Delta T \doteq \Delta x_i/v_i. \tag{19}$$

Good energy conservation during a timestep ultimately depends upon the change in force during the timestep. Once the maximum acceptable force change is assumed, the displacement which will produce that change is readily computed. Call this maximum acceptable displacement D. In these computations it is simple to determine the body with largest kinetic energy T_m at the end of each timestep. Then from

Eq. (19) we define

$$\Delta T = D(2m/T_m)^{-\frac{1}{2}}. \tag{20}$$

There are two safety factors built into this definition of ΔT:

(1) it is based upon the most energetic body, so the single timestep displacements of all other bodies will be less than D, and

(2) only very rarely will the velocity of the most energetic body be parallel to a coordinate axis; so generally any component of its displacement will be less than D.

In cubic lattices the *lattice unit* (LU), where 1 LU = $\frac{1}{2}a_0$, the cubic lattice parameter, is a convenient length unit. We have empirically determined that all $D < 0.1$ LU give essentially the same trajectories and energy decrements of the order of 1% for a system of 50 or more bodies and 250 timesteps. Smaller values of D decrease the energy decrement, but do not affect the trajectories very much. In comparison, $D = 0.2$ LU may give decrements as large as 10% after only 25 timesteps.

In lattice-relaxation studies, we sometimes deal with systems where $v \ll \langle F_i \rangle / 2m$. When this is the case, we determine the maximum force acting on any body F_m and define

$$\Delta T = (2mD/F_m)^{\frac{1}{2}}. \tag{21}$$

Although this is the most satisfactory approach discovered to date, Eq. (21) can lead to large errors if finite-range forces, or potentials, are used in the system.

VI. FINITE-RANGE POTENTIALS

In the numerical integration of the equations of motion for large numbers of interacting bodies, it is usually not practical to include long-range forces. We have performed computations which reach to the fifth nearest-neighbor in the face-centered cubic lattice (~3.4 LU) where each body may interact with as many as 64 of its neighbors. Even with an IBM 300/67 this is impractical except for an occasional special case, and interaction ranges $R < 2.0$ LU, which involve only 18 other atoms, are more realistic.

For this reason, every computation must include a means of carrying out the integration of the equations of motion for timesteps in which the force "turns on" in the middle of the timestep. The method outlined below is feasible with the AF algorithm and has been found to significantly improve the energy conservation, that is, reduce the energy decrement, in all cases tested to date.

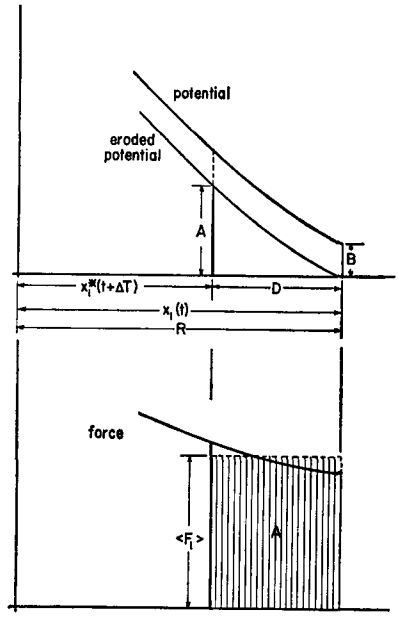

FIG. 4. When the force "turns on" just at the beginning of the timestep, the AF method computes the change in potential energy, A in each diagram, quite accurately.

With short-range potential functions it is often more convenient to truncate mathematically the potential at some separation R, the range, than to construct a function which vanishes at this separation. When $V(r)$ is truncated at R, so that $V(R)$ is finite, we can shift the zero of potential by an amount $V(R)$ and define an *eroded potential*

$$V_e(r) \equiv V(r) - V(R)$$

which vanishes at $r = R$. This charge does not affect the force $F(r) = -\nabla V(r) = -\nabla V_e(r)$, for $r < R$, but it too must be truncated at $r = R$. The difficulties introduced by the "turning on" of the force at $r = R$ occur whether $V(r)$ is truncated or not.

Let us now examine a single binary-collision event in detail. In Fig. 4, the bodies have just made contact at the end of the last timestep. We are concerned with the preliminary displacement $x_i^*(t + \Delta T)$, because we would like the definition of $\langle F_i \rangle$ to compensate for the "turn on" process. On both the potential and force diagrams of Fig. 4, A is the work done during the preliminary displacement and $x_i^*(t + \Delta T)$ is approximately the final separation at the end of the timestep. Under these conditions the normal definition of $\langle F_i \rangle$ by Eq. (14) introduces no difficulties.

Now consider the situation shown in Fig. 5. We note that the CD method is completely unsuitable, because it would assume zero force for the entire timestep. The average force as defined by Eq. (14) is somewhat more realistic, but the AF integration may also contain significant errors in the approximate integration.

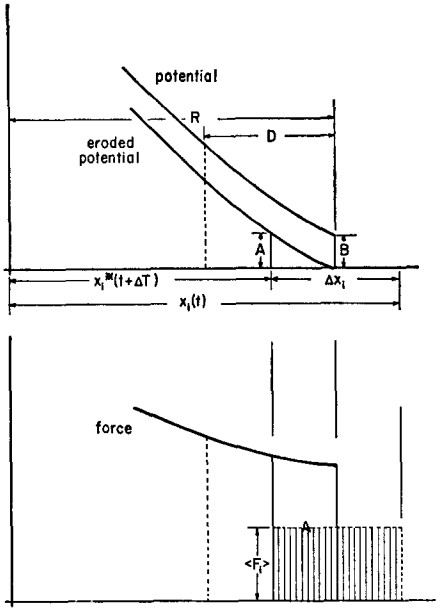

FIG. 5. When the force "turns on" during the timestep, we determine a first approximation to A from the change in potential energy, and then define $\langle F_i \rangle \equiv A/\Delta x_i$.

We can make a better approximation to $\langle F_i \rangle$ under these conditions if we note that $x_i^*(t + \Delta T)$ is approximately the final separation, so $V(x_i^*)$ should be approximately the final potential energy. Energy will be approximately conserved if the work done by the body during the timestep approximately equals the charge in potential energy. This requires that

$$\langle F_i \rangle \Delta x_i = A. \tag{22}$$

This is immediately accomplished if we define

$$\langle F_i \rangle = -\frac{V(x_i^*) - V(R)}{x_i^* - R}, \quad R - D < x_i^* < R,$$

where D is the maximum displacement defined in the last section. If the potential is eroded, this reduces to

$$\langle F_i \rangle = -\frac{V_e(x_i^*)}{x_i^* - R}, \quad R - D < x_i^* < R.$$

Programs run with this modification have a smaller energy decrement than identical situations run as an unmodified AF integration. The improvement is particularly noticeable in test cases which approach the assumed limits of the AF-method approximations.

VII. SUMMARY

We have shown that it is possible to carry out the numerical integration of the classical equations of motion for N bodies by an average-force algorithm and have shown that this algorithm has both theoretical and practical advantages when compared with the central-difference algorithm which is currently in general use.

Wave Equations, Multipole Solutions, and Characteristic Hypersurfaces for Massless Particles*

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(Received 28 July 1968)

In this paper, the canonical wave equation and auxiliary conditions for a massless particle with arbitrary integral or half-integral spin s are derived from a symmetric spinor formulation. The wave equation is solved for the multipole solutions using the appropriate parity operator for each spin. Finally, the characteristic hypersurfaces for the wave equation are derived and found to agree with that of the photon. The special cases of spins one, three-halves, and two are detailed in conclusion.

I. INTRODUCTION

It is well known[1] that one can write Maxwell's equations for the photon as a simple matrix equation and auxiliary condition. The equation is (the units are $\hbar = c = 1$):

$$\bar{\mathbf{S}} \cdot \mathbf{P}\bar{\psi}(x) = i\frac{\partial}{\partial t}\bar{\psi}(x), \tag{1}$$

where $\bar{\psi}(x)$ is a three-component wavefunction with elements

$$\bar{\psi}_k = \mathfrak{E}_k + i\mathfrak{B}_k \tag{2}$$

and $\mathbf{P}$ is $-i\nabla$. $\mathfrak{E}$ and $\mathfrak{B}$ are the (real) electric and magnetic fields and $x = (\mathbf{x}, it)$. The $\bar{\mathbf{S}}$ are the representations of spin-one matrices

$$(\bar{S}_i)_{jk} = -i\epsilon_{ijk}. \tag{3}$$

The auxiliary condition specifying the transverse nature of the electric and magnetic fields may be written as

$$\frac{\partial}{\partial x_k}\bar{\psi}_k(x) = 0. \tag{4}$$

This condition insures that the photon wavefunction contains only helicity components ± 1 as is required for a massless particle.[2]

The construction of the above theory for the photon follows from a symmetric spinor formulation of the theory of a free particle with arbitrary mass and spin[3] specialized to zero mass. In particular, for spin one, the spinor equations are

$$\partial^{\alpha\beta_1}\phi_{\beta_1\beta_2}(x) = 0, \tag{5}$$

where $\phi_{\beta_1\beta_2}$ is a lower-dotted symmetric two-index spinor and α, β_1, β_2 run from 1 to 2, so there are only three independent components which are labeled according to

$$\phi_{\dot{1}\dot{1}} \equiv \chi_0, \quad \phi_{\dot{2}\dot{1}} \equiv \chi_1, \quad \phi_{\dot{2}\dot{2}} \equiv \chi_2. \tag{6}$$

The mixed-index spinor $\partial^{\alpha\beta_1}$ is related to the four-vector gradient $\partial/\partial x_\mu$ by

$$\partial^{\alpha\beta_1} = -(\sigma_\mu)_{\alpha\beta_1}\frac{\partial}{\partial x_\mu}, \tag{7}$$

where, except for α and $\beta_1, \beta_2, \cdots$, the Greek indices run from 1 to 4 and where the σ_i are the Pauli matrices and σ_4 is i times the 2×2 identity. The four equations (5) can be written in the form

$$\left[\boldsymbol{\sigma}\cdot\nabla + \frac{\partial}{\partial t}\right]\begin{bmatrix}\chi_0\\ \chi_1\end{bmatrix} = 0,$$
$$\left[\boldsymbol{\sigma}\cdot\nabla + \frac{\partial}{\partial t}\right]\begin{bmatrix}\chi_1\\ \chi_2\end{bmatrix} = 0. \tag{8}$$

If one now defines the wavefunction ψ with three components given by

$$\psi_k = \left[\binom{2}{k-1}\right]^{\frac{1}{2}}\chi_{k-1}, \quad k = 1, 2, 3, \tag{9}$$

where

$$\binom{m}{n} = \frac{m!}{n!\,(m-n)!}, \tag{10}$$

then Eqs. (8) can be written as

$$\mathbf{S}\cdot\mathbf{P}\psi(x) = i\frac{\partial}{\partial t}\psi(x), \tag{11}$$

where the $\mathbf{S}$ are the spin-one matrices in a representation with S_3 diagonal. There are four equations (8) and only three equation (7), so the remaining equation is considered an auxiliary condition on ψ. The auxiliary condition takes the form

$$\left(\frac{\partial}{\partial x_1} + i\frac{\partial}{\partial x_2}\right)\psi_1 - \sqrt{2}\frac{\partial}{\partial x_3}\psi_2 - \left(\frac{\partial}{\partial x_1} - i\frac{\partial}{\partial x_2}\right)\psi_3 = 0. \tag{12}$$

* Work supported in part by the U.S. Atomic Energy Commission.

[1] R. H. Good, Jr., Phys. Rev. **105**, 1914 (1957). This paper contains earlier references on the subject.

[2] E. P. Wigner, Rev. Mod. Phys. **29**, 255 (1957).

[3] D. L. Weaver and D. M. Fradkin, Nuovo Cimento **37**, 440 (1965). The spinor notation of this paper is followed.

Equations (1)–(4) may be reproduced by noting that

$$\bar{\psi} = U\psi, \tag{13}$$

where

$$U = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & -1 \\ i & 0 & i \\ 0 & -\sqrt{2} & 0 \end{bmatrix}, \quad U^{-1} = U^{\dagger}, \tag{14}$$

and

$$\bar{\mathbf{S}} = USU^{\dagger}. \tag{15}$$

The above considerations for spin one may be carried out for arbitrary integral or half-integral spin and zero mass and this is done in Sec. II to yield the wave equation for a massless particle with arbitrary spin previously discussed by Hammer and Good.[4] In Sec. III this wave equation is used to solve the multipole-radiation problem for arbitrary spin, and the eigenstates of the two types of parity operators for massless particles are constructed. The characteristic hypersurfaces are found in Sec. IV and some special cases are discussed in Sec. V.

II. WAVE EQUATION FORMULATION

The construction for spin one may be extended to the general case. The spinor equations are

$$\partial^{\alpha\dot{\beta}_1}\phi_{\beta_1\beta_2\cdots\beta_{2s}} = 0, \tag{16}$$

where ϕ is completely symmetric and so has $2s+1$ independent components. Note that the identity

$$\partial_{\alpha\dot{\beta}}\partial^{\alpha\dot{\beta}_1} = -\delta_{\beta\dot{\beta}_1}\frac{\partial}{\partial x_\mu}\frac{\partial}{\partial x_\mu} \tag{17}$$

together with Eq. (16) shows that each component of the spinor satisfies the equation

$$\left[\nabla^2 - \frac{\partial^2}{\partial t^2}\right]\phi_{\beta_1\cdots\beta_{2s}} = 0. \tag{18}$$

The $2s+1$ independent components of ϕ are defined by

$$\chi_0 \equiv \phi_{\dot{1}\dot{1}\cdots\dot{1}}, \quad \chi_1 \equiv \phi_{\dot{2}\dot{1}\cdots\dot{1}}, \cdots, \chi_{2s} = \phi_{\dot{2}\dot{2}\cdots\dot{2}}. \tag{19}$$

One can rewrite the 2^{2s} equations (16) in the form

$$\left[\boldsymbol{\sigma}\cdot\nabla + \frac{\partial}{\partial t}\right]\begin{pmatrix}\chi_{n-1}\\ \chi_n\end{pmatrix} = 0, \quad n = 1, 2, \cdots, 2s, \tag{20}$$

which is a set of $4s$ coupled, linear, homogeneous first-order differential equations for the independent components. There are, in addition, $2^{2s} - 4s$ equations which are identical to some of Eqs. (20). Defining the wavefunction ψ with $2s+1$ components by

$$\psi_k = \left[\binom{2s}{k-1}\right]^{\frac{1}{2}}\chi_{k-1}, \quad k = 1, 2, \cdots, 2s, \tag{21}$$

one may rewrite Eqs. (20) as

$$\frac{1}{s}\mathbf{S}\cdot\mathbf{P}\psi(x) = i\frac{\partial}{\partial t}\psi(x) \tag{22}$$

and

$$\left[\binom{2s}{k-1}\right]^{-\frac{1}{2}}\left(\frac{\partial}{\partial x_1} + i\frac{\partial}{\partial x_2}\right)\psi_k - 2\left[\binom{2s}{k}\right]^{-\frac{1}{2}}\frac{\partial}{\partial x_3}\psi_{k+1} - \left[\binom{2s}{k+1}\right]^{-\frac{1}{2}}\left(\frac{\partial}{\partial x_1} - i\frac{\partial}{\partial x_2}\right)\psi_{k+2} = 0 \tag{23}$$

with $k = 1, 2, \cdots, 2s-1$ here. Now, the $\mathbf{S}$ are the $(2s+1)$-dimensional spin matrices in a representation with S_3 diagonal. Equation (22) is the wave equation discussed by Hammer and Good.[4] One may see the effect of the auxiliary conditions (23) very clearly by considering for ψ a plane-wave solution propagating in the z direction:

$$\psi(x) = U(\mathbf{P})\exp\left[i(P_3 z - Et)\right]. \tag{24}$$

Then the auxiliary conditions state that $U(\mathbf{P})$ represents a physical state only if $[U(\mathbf{P})]_n = 0$, for $n = 2, 3, \cdots, 2s$. Thus, physical states are represented by $U(\mathbf{P}) = \{[U(\mathbf{P})]_1, 0, \cdots, [U(\mathbf{P})]_{2s+1}\}$, the two linearly independent solutions $[U(\mathbf{P})]_1 = 1$, $[U(\mathbf{P})]_{2s+1} = 0$, and $[U(\mathbf{P})]_1 = 0$, $[U(\mathbf{P})]_{2s+1} = 1$, corresponding to $E = +|P_3|$ and $E = -|P_3|$, respectively.

Some results taken over without any proof from Ref. 4 are that KCP is the space-reflection operator for ψ and that $\mathbf{J}$ is the total-angular-momentum operator, where

$$K\psi(\mathbf{x}, t) = \psi^*(\mathbf{x}, t), \tag{25}$$

$$P\psi(\mathbf{x}, t) = \psi(-\mathbf{x}, t), \tag{26}$$

$$CSC^{-1} = -\mathbf{S}^*, \tag{27}$$

$$(KCP)^2 = (-1)^{2s}, \tag{28}$$

and

$$J_i = \epsilon_{ijk}x_j\left(-i\frac{\partial}{\partial x_k}\right) + S_i. \tag{29}$$

III. MULTIPOLE SOLUTIONS

The problem to be solved in this section is to find solutions $\psi(\mathbf{x}, t)$ which have a definite, nonzero frequency, which satisfy Eq. (22) everywhere except at the origin and which, far from the origin, are outgoing waves. One may write

$$\psi(\mathbf{x}, t) = w(\mathbf{x})\exp(-iEt), \tag{30}$$

so that

$$s^{-1}\mathbf{S}\cdot\mathbf{P}w(\mathbf{x}) \equiv Hw(\mathbf{x}) = Ew(\mathbf{x}) \tag{31}$$

[4] C. L. Hammer and R. H. Good, Jr., Phys. Rev. **108**, 882 (1957).

for the corresponding eigenvalue problem. The eigenvalue E must be nonzero and $w(\mathbf{x})$ must behave correctly, asymptotically, so that $\psi(\mathbf{x}, t)$ becomes an outgoing wave. One wants to find the common eigenfunctions of the commuting set of operations H, S^2, J^2, J_3. The simultaneous eigenfunctions of J^2, S^2, and J_3 are the spinor spherical harmonics $\Psi^M_{J,l,s}(\theta, \varphi)$ which satisfy the equations

$$J^2\Psi^M_{J,l,s} = J(J+1)\Psi^M_{J,l,s}, \tag{32}$$

$$J_3\Psi^M_{J,l,s} = M\Psi^M_{J,l,s}, \tag{33}$$

and

$$S^2\Psi^M_{J,l,s} = s(s+1)\Psi^M_{J,l,s}, \tag{34}$$

where J^2, J_3, and S^2 on the left are operators and J and s on the right and in the subscripts form the eigenvalue. For spin one, the $\Psi^M_{J,l,1}$ are the vector spherical harmonics as given, for example, by Blatt and Weisskopf[5] and in general, the spinor spherical harmonics are defined by

$$\Psi^M_{J,l,s}(\theta, \varphi) = \sum_{m_l+m_s=M} (lm_lsm_s \mid JlsM) Y_{l,m_l}(\theta, \varphi) \mid s, m_s\rangle, \tag{35}$$

where Y_{l,m_l} are spherical harmonics and $\mid s, m_s\rangle$ are the $(2s+1)$-dimensional eigenvectors of S^2 and S_3. (See Appendix A for some properties of these functions.) The $(lm_lsm_s \mid JlsM)$ are Clebsch–Gordan coefficients[6] and have the symmetry property

$$(lm_lsm_s \mid JlsM) = (-1)^{l+s-J}(l - m_ls - m_s \mid Jls - M). \tag{36}$$

The quantum number J is always greater than or equal to s and otherwise can take the values s, $s+1, \cdots$; M may be any of the $2J+1$ values $-J$, $-J+1, \cdots, J$; l is an integer in the range $J - s \leq l \leq J + s$. The reason for $J \geq s$ is discussed in Appendix B.

One weighs each spinor spherical harmonic with a radial function and makes the substitution

$$w^s_{E,J,M}(\mathbf{x}) = \sum_{l=J-s}^{J+s} h_l(r)\Psi^M_{J,l,s}(\theta, \varphi) \tag{37}$$

into Eq. (31) where the $2s+1$ radial functions (with the other indices suppressed) are to be determined.

Using the formulas of Hill[7] for the derivatives of radial functions times spherical harmonics, Eq. (31) gives the equations for the radial functions:

$$(i/2s)a^{J,s}_{J-s}d^{J-s+2}_+(h_{J-s+1}) = Eh_{J-s}, \tag{38}$$

$$(i/2s)a^{J,s}_{J+s-1}d^{J+s-1}_-(h_{J+s-1}) = Eh_{J+s}, \tag{39}$$

$$(i/2s)[a^{J,s}_{l-1}d^{l-1}_-(h_{l-1}) + a^{J,s}_l d^{l+2}_+(h_{l+1})] = Eh_l, \tag{40}$$

where $J - s + 1 \leq l \leq J + s - 1$. The coefficients $a^{J,s}_l$ are defined by

$$a^{J,s}_l \equiv \left[\frac{(l+s+J+2)(l+s-J+1)(l-s+J+1)(J+s-l)}{(2l+1)(2l+3)}\right]^{\frac{1}{2}} \tag{41}$$

and

$$d^l_\pm \equiv d/(dr) \pm l/r. \tag{42}$$

The solutions of the radial equations are found to be

$$h^{(1,2)}_l(r) = (C_l/\rho^{\frac{1}{2}})H^{(1,2)}_{l+\frac{1}{2}}(\rho), \tag{43}$$

where

$$\rho \equiv |E|\, r \tag{44}$$

and $H^{(1)}$, $H^{(2)}$ are the first, second Hankel functions, respectively, in the notation of Jahnke and Emde.[8] To get outgoing waves one uses the first Hankel function when E is positive and the second when E is negative. One uses the recursion relation of the Hankel functions

$$\frac{n}{\rho}H^{(1,2)}_n(\rho) = H^{(1,2)}_{n-1}(\rho) - \frac{d}{d\rho}H^{(1,2)}_n(\rho) = H^{(1,2)}_{n+1}(\rho) + \frac{d}{d\rho}H^{(1,2)}_n(\rho) \tag{45}$$

to get the relations

$$d^n_-(\rho^{-\frac{1}{2}}H^{(1,2)}_{n+\frac{1}{2}}(\rho)) = -\rho^{-\frac{1}{2}}H^{(1,2)}_{n+\frac{3}{2}}(\rho), \tag{46}$$

$$d^n_+(\rho^{-\frac{1}{2}}H^{(1,2)}_{n-\frac{1}{2}}(\rho)) = \rho^{-\frac{1}{2}}H^{(1,2)}_{n-\frac{3}{2}}(\rho). \tag{47}$$

Substituting Eq. (43) into Eqs. (38), (39), and (40), and using the relations (46) and (47), one finds the following equations for the C_l:

$$(i/2s)a^{J,s}_{J-s}C_{J-s+1} = \epsilon C_{J-s}, \tag{48}$$

$$-(i/2s)a^{J,s}_{J+s-1}C_{J+s-1} = \epsilon C_{J+s}, \tag{49}$$

and

$$(i/2s)[-a^{J,s}_{l-1}C_{l-1} + a^{J,s}_l C_{l+1}] = \epsilon C_l. \tag{50}$$

[5] J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, New York, 1952), Appendix B.

[6] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, N.J., 1957).

[7] E. L. Hill, Am. J. Phys. **22**, 211 (1954).

[8] E. Jahnke and F. Emde, *Tables of Functions* (Dover Publications, New York, 1945), Chap. VIII.

One solves these equations for the C_l in the cases of interest, where ϵ is equal to $E/|E|$.

The solutions of Eq. (31) are then given by

$$\psi(\mathbf{x}, t) = \sum_{l=J-s}^{J+s} C_l \rho^{-\frac{1}{2}} H^{(1,2)}_{l+\frac{1}{2}}(\rho) \Psi^M_{J,l,s}(\theta, \varphi) e^{-iEt}. \quad (51)$$

For large values of its argument, $H^{(1,2)}$ behaves like $\rho^{-\frac{1}{2}} e^{\pm i\rho}$. To get outgoing waves, the first Hankel function is to be used when E is positive and the second when E is negative. The complete solutions to the problem are then

$$\psi^{\pm}(J, M, s, |E|; \mathbf{x}, t) = \sum_{l=J-s}^{J+s} C_l \rho^{-\frac{1}{2}} H^{(1,2)}_{l+\frac{1}{2}}(\rho) \Psi^M_{J,l,s} \exp(\mp i |E| t). \quad (52)$$

The upper (lower) signs are for positive (negative) E solutions and the first (second) kind of Hankel function is to be used with them.

In analogy with the photon, the definite-parity solutions (the "electric" and "magnetic" multipole solutions) are given for the integral-spin theories by

$$\psi_{\text{mag}}(J, M, s, |E|; \mathbf{x}, t) = \psi^{+} + (-1)^J KCP\psi^{+}, \quad (53)$$

$$\psi_{\text{elec}}(J, M, s, |E|; \mathbf{x}, t) = i\psi_{\text{mag}}(J, M, s, |E|; \mathbf{x}, t), \quad (54)$$

where the operators K, C, and P are defined in Eqs. (25), (26), and (27). Using Appendix A, one sees that the effect for any spin of operating with KCP on $\psi^{\pm}$ is

$$KCP\psi^{\pm}(J, M, s, |E|; \mathbf{x}, t) = (i)^{2(s-J+M)} \psi^{\mp}(J, -M, s, |E|). \quad (55)$$

The motivation for the form of Eqs. (53) and (54) is that

$$KCP\psi_{\text{mag}} = (-1)^J \psi_{\text{mag}}, \quad (56)$$

$$KCP\psi_{\text{elec}} = (-1)^{J+1} \psi_{\text{elec}}, \quad (57)$$

and that for spin one the solutions are identical (up to the representation of spin matrices) to those discussed in detail for the photon by Good.[9] For the half-integer spin theories, the linear combinations of Eqs. (53) and (54) do not give definite parity solutions. In fact, one must use, for the half-integral spin theories, instead of KCP, the operator $KCP(H/|H|)$. With this operator one has, for the half-integer spin theories, the eigenstates $\tilde{\psi}_{\text{mag}}$ and $\tilde{\psi}_{\text{elec}}$, where

$$\tilde{\psi}_{\text{mag}} = \psi^{+} + (-1)^{J-\frac{1}{2}} KCP(H/|H|)\psi^{+}, \quad (58)$$

$$\tilde{\psi}_{\text{elec}} = i\tilde{\psi}_{\text{mag}}, \quad (59)$$

and

$$KCP(H/|H|)\tilde{\psi}_{\text{mag}} = (-1)^{J-\frac{1}{2}} \tilde{\psi}_{\text{mag}}, \quad (60)$$

$$KCP(H/|H|)\tilde{\psi}_{\text{elec}} = (-1)^{J+\frac{1}{2}} \tilde{\psi}_{\text{elec}}. \quad (61)$$

The two possibilities for the parity operator for massless particles correspond to the duality of charge-conjugation operations discussed recently by Weaver.[10]

IV. CHARACTERISTIC HYPERSURFACES

In this section the problem considered is that of finding the characteristic hypersurfaces associated with the wave equation (22) for massless particles with arbitrary spin. The physical motivation for considering such hypersurfaces is discussed, for example, in Ref. 11. The problem is to find the hypersurfaces over which a discontinuity can occur in the first derivatives of the solutions of the wave equation.

Let h be any hypersurface given by

$$t = f(\mathbf{x}) \quad (62)$$

and let $\tilde{\psi}$ be ψ, the solution of the wave equation restricted to h, so that

$$\tilde{\psi}(\mathbf{x}) = \psi(\mathbf{x}, f). \quad (63)$$

Then, on h, one has

$$\frac{\partial}{\partial x_i} \tilde{\psi} = \frac{\partial}{\partial x_i} \psi + \frac{\partial f}{\partial x_i} \frac{\partial}{\partial t} \tilde{\psi} \quad (64)$$

and so

$$\frac{1}{s} \mathbf{S} \cdot \mathbf{P} \tilde{\psi} = \frac{1}{s} \mathbf{S} \cdot \mathbf{P} \psi + \left(\frac{1}{is} \mathbf{S} \cdot \nabla f \right) \frac{\partial}{\partial t} \psi. \quad (65)$$

Making use of the wave equation, one reduces Eq. (65) to

$$\frac{1}{s} \mathbf{S} \cdot \mathbf{P} \tilde{\psi} = i \left(1 - \frac{1}{s} \mathbf{S} \cdot \nabla f \right) \frac{\partial}{\partial t} \psi. \quad (66)$$

One must consider two cases. First, if the determinant of $1 - s^{-1}\mathbf{S} \cdot \nabla f \neq 0$, then the inverse exists and one may calculate $(\partial/\partial t)\psi$, $(\partial^2/\partial t^2)\psi$, etc., in terms of initial data and so in this case h is not a characteristic hypersurface. The second and most interesting case is when the determinant is zero. Then h is a characteristic hypersurface, the equation being

$$\det(1 - s^{-1}\mathbf{S} \cdot \nabla f) = 0. \quad (67)$$

For spin one, this gives the equation

$$(\nabla f) \cdot (\nabla f) = 1, \quad (68)$$

which is the equation of the characteristic hypersurfaces for Maxwell's equations. For arbitrary spin, one

[9] R. H. Good, Jr., Ann. Phys. (N.Y.) **1**, 213 (1957).

[10] D. L. Weaver, Nuovo Cimento **55A**, 377 (1968).

[11] R. Adler, M. Bazin, and M. Schiffer, *Introduction to General Relativity* (McGraw-Hill Book Co., New York, 1965).

gets

$$\det(1 - s^{-1}\mathbf{S}\cdot\nabla f) \propto [(\nabla f)^2 - 1] \times \{(\nabla f)^2 - [s/(s-1)]^2\}\cdots[(\nabla f)^2 - (s/\epsilon_s)^2], \quad (69)$$

where $\epsilon_s = \frac{1}{2}(1)$ for $s =$ half-integer (integer). So for h to be a characteristic hypersurface, one finds that f must satisfy

$$\prod_{m=\epsilon_s}^{s}\left[(\nabla f)^2 - \left(\frac{s}{m}\right)^2\right] = 0. \quad (70)$$

For $s = \frac{1}{2}$, 1, there is only one possibility, which is Eq. (68). For higher spins, one gets equations of the form

$$(\nabla f)^2 - \beta^{-2} = 0, \quad (71)$$

where

$$\beta = (m/s) \leq 1. \quad (72)$$

The basic solution of Eq. (71) is

$$f = \frac{1}{\beta}\left[\sum_{i=1}^{3}(x_i - a_i)^2\right]^{\frac{1}{2}} \quad (73)$$

and h is then given by

$$t - t_0 = \frac{1}{\beta}\left[\sum_{i=1}^{3}(x_i - a_i)^2\right]^{\frac{1}{2}} \quad (74)$$

or, equivalently, by

$$\beta^2(t - t_0)^2 - \sum_{i=1}^{3}(x_i - a_i)^2 = 0, \quad (75)$$

which corresponds to a spherical wavefront expanding with velocity βc. The extra hypersurfaces, those corresponding to $\beta < 1$, are not allowed by the auxiliary conditions (23) which together with Eq. (22) form a complete theory. One may easily see this by finding the characteristic hypersurfaces of Eqs. (20). One finds only the surfaces with $\beta = 1$, as expected.

V. SPECIAL CASES

We list here the radial functions for spins 1, $\frac{3}{2}$, 2. Results for spins 1 (photon) and 2 (graviton) agree with those of Refs. 12 and 13:

Spin $= 1$:

$$h^{(k)}_{J+1} = \epsilon J^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J+\frac{3}{2}},$$
$$h^{(k)}_{J} = i(2J+1)^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J+\frac{1}{2}},$$
$$h^{(k)}_{J-1} = -\epsilon(J+1)^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J-\frac{1}{2}}.$$

Spin $= \frac{3}{2}$:

$$h^{(k)}_{J-\frac{3}{2}} = \epsilon[3(J+1)]^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J-1},$$
$$h^{(k)}_{J-\frac{1}{2}} = -3iJ^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J},$$
$$h^{(k)}_{J+\frac{1}{2}} = -3\epsilon\left[\frac{(2J-1)(J+1)}{2J+3}\right]^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J+1},$$
$$h^{(k)}_{J+\frac{3}{2}} = i\left[\frac{3J(2J-1)}{2J+3}\right]^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J+2}.$$

Spin $= 2$:

$$h^{(k)}_{J+2} = \epsilon(2J)^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J+\frac{5}{2}},$$
$$h^{(k)}_{J+1} = 2i(2J+3)^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J+\frac{3}{2}},$$
$$h^{(k)}_{J} = -6\epsilon\left[\frac{(2J+1)(J+2)}{3(2J-1)}\right]^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J+\frac{1}{2}},$$
$$h^{(k)}_{J-1} = -2i\left[\frac{(J+2)(2J+3)}{(J-1)}\right]^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J-\frac{1}{2}},$$
$$h^{(k)}_{J-2} = \epsilon\left[\frac{2(J+1)(J+2)(2J+3)}{(J-1)(2J-1)}\right]^{\frac{1}{2}}\rho^{-\frac{1}{2}}H^{(k)}_{J-\frac{3}{2}}.$$

We note that for solutions regular at the origin one replaces the Hankel function by Bessel's function of equal degree.

APPENDIX A: PROPERTIES OF THE OPERATORS AND EIGENFUNCTIONS

In the representation with S_3 diagonal, the spin matrices have elements

$$(S_1)_{m+1,m} = (S_1)_{m,m+1} = \tfrac{1}{2}[(s-m)(s+m+1)]^{\frac{1}{2}}, \quad (A1)$$

$$(S_2)_{m+1,m} = -(S_2)_{m,m+1} = -\tfrac{1}{2}i[(s-m)(s+m+1)]^{\frac{1}{2}}, \quad (A2)$$

$$(S_3)_{m,m} = m, \quad (A3)$$

where m ranges from $-s$ to s in integral steps and the elements not listed are zero. In this representation, the matrix C has elements

$$C_{mn} = (i)^{2m}\delta_{m,-n}, \quad (A4)$$

C is Hermitian and unitary, and has the further properties

$$C^2 = 1, \quad (A5)$$

$$C^*C = CC^* = (-1)^{2s}. \quad (A6)$$

The eigenfunctions of S^2 and S_3 are

$$(|s, m\rangle)_n = \delta_{mn}, \quad (A7)$$

and they have the properties

$$C\,|s, m\rangle = (-i)^{2m}\,|s, -m\rangle, \quad (A8)$$

$$P\,|s, m\rangle = |s, m\rangle. \quad (A9)$$

The spherical harmonics have the properties

$$KY_{l,m_l} = (-1)^{m_l}Y_{l,-m_l}, \quad (A10)$$

$$PY_{l,m_l} = (-1)^lY_{l,m_l}. \quad (A11)$$

Combining the above properties, one finds for the spinor spherical harmonics

$$KC\Psi^M_{J,l,s} = (-1)^{l+s+M-J}\Psi^{s-M}_{J,l,s}, \quad (A12)$$

$$P\Psi^M_{J,l,s} = (-1)^l\Psi^M_{J,l,s}. \quad (A13)$$

[12] R. H. Good, Jr., *Lectures in Theoretical Physics* (University of Colorado Press, Boulder, Colo., 1958), Vol. 1.

[13] L. Halpern and B. Laurent, Nuovo Cimento **33**, 728 (1964).

With respect to complex conjugation, the Hankel functions have the property

$$KH^{(1,2)}_{l+\frac{1}{2}}(\rho) = H^{(2,1)}_{l+\frac{1}{2}}(\rho). \tag{A14}$$

APPENDIX B: ON EXISTENCE OF PHYSICAL SOLUTIONS

We give here a brief discussion of the solutions of Eq. (31).

Conditions (23) imply that for a solution of wave equation (22) to be physically acceptable, it must satisfy the Klein–Gordon equation. Thus, $w^s_{E,J,M}$ is physically acceptable if it satisfies

$$-\nabla^2 w^s_{E,J,M} = E^2 w^s_{E,J,M}.$$

Now, making the substitution

$$h_{l,\alpha}(r) \equiv \frac{C_l}{\rho^{\frac{1}{2}}} H_{l+\frac{1}{2}}(\alpha\rho) \tag{B1}$$

in Eqs. (38)–(40), one finds that the determinant of the unknowns C_l is given by

$$D_{J,s}(\alpha) = (-\epsilon)^{k+1} \times \left[1 + \alpha^2 \sum_{r=1}^{k} a_r^2 + \alpha^4 \sum_{r_1+2\le r_2} a_{r_1}^2 a_{r_2}^2 + \cdots\right], \tag{B2}$$

where

$$k = J + s - |J - s|, \quad a_r \equiv \frac{i}{2s} a^{J,s}_{|J-s|+r-1}.$$

Now it can be shown that the roots of $D_{J,s}(\alpha)$ are real and that $\alpha = \pm 1$ is a root only if $J \geq s$. Now since

$$w(\mathbf{x}) = \sum_{l=|J-s|}^{J+s} h_{l,\alpha}(r) \Psi^M_{J,l,s}$$

satisfies

$$-\nabla^2 w = \alpha^2 E^2 w,$$

one sees that physically acceptable radiative solutions exist and are given by (B1), only for $J \geq s$. This is the range assumed, therefore, in the paper.

The equivalence of the Klein–Gordon equation and the auxiliary conditions (23) can be seen as follows.

The most general solution of wave equation (22) is

$$\psi(\mathbf{x}, t) = \int d\mathbf{P} \sum_{m=-s}^{s} A_m(\mathbf{P}) U_m(\mathbf{P}) \times \exp\left[i\left(\mathbf{P}\cdot\mathbf{x} - \frac{m}{s}|E|\, t\right)\right], \tag{B3}$$

where $U_m(\mathbf{P})$ are the orthonormal eigenvectors of the helicity operator $|\mathbf{P}|^{-1}\, \mathbf{S}\cdot\mathbf{P}$. Now the requirement

$$\left[-\nabla^2 + \frac{\partial^2}{\partial t^2}\right]\psi(\mathbf{x}, t) = 0$$

leads to

$$A_m(\mathbf{P}) = 0, \quad -s < m < s$$

and so only states of helicity ± 1 contribute in (B3), which is precisely what the auxiliary condition (23) amounts to, as argued in the paper.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

On the Width Distribution for a Complex System Whose Hamiltonian Contains a Small Interaction That Is Odd under Time-Reversal*

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(Received 13 August 1968)

An approximate expression for the width distribution of a complex system with a small odd term is given. The expression is compared with available Monte-Carlo calculations and seems to be a good approximation for large N ($10 \leq N \leq 100$).

1. INTRODUCTION

A question of current interest[1,2] is whether or not the presence of a small time-reversal odd term in the Hamiltonian of a complex system, such as a heavy nucleus, will manifest itself in various statistical properties in an observable manner. It has been shown that effects on the nearest-neighbor spacing distribution are such that their experimental observation seems extremely difficult.[1,2]

There has been little progress made in the analytic calculation of the distribution of widths for an odd term of arbitrary size,[3] although some Monte-Carlo calculations have been carried out.[1] We have obtained an explicit expression for a Gaussian ensemble when $N = 2$ (N = dimension of the Hamiltonian submatrix with a fixed set of quantum numbers). We were not able to carry out an analytical calculation for arbitrary N.[4] However, from our results for $N = 2$ and the known results for the limiting cases [i.e., the odd term is zero (orthogonal ensemble) and the odd term is of the same size as the even term (unitary ensemble)] a form is conjectured which we believe to be at least a good approximation when the odd term is very small and $N \gg 1$. We have compared this distribution with the available Monte-Carlo results and found it to approximate them quite well.

An interesting feature of our distribution is that, in the limit as $N \to \infty$, it approaches one of three limits, depending on the ratio of the odd to the even term. Only if the ratio goes to zero as $1/N$ is the limiting distribution different from the orthogonal or unitary result.

2. THE ENSEMBLE AND DISTRIBUTION OF WIDTHS

The distribution of matrix elements is chosen to be[5]

$$p_N(H, \gamma, \alpha) = \eta \exp(-\alpha \operatorname{Tr} H^2) \exp\left(-2\gamma \sum_{i>j} S_{ij}^2\right), \tag{1}$$

where

$$\eta = 2^{N(N-1)/2}(\alpha/\pi)^{N(N+1)/4}[(\alpha + \gamma)/\pi]^{N(N-1)/4} \tag{2}$$

and

$$H_{ij} = R_{ij} + iS_{ij}. \tag{3}$$

Since the Hamiltonian matrix H is Hermitian,

$$R_{ij} = R_{ji} \tag{4}$$

and

$$S_{ij} = -S_{ji}, \tag{5}$$

where R and S are both real matrices. Note that, for $\gamma \to \infty$, p_N becomes the orthogonal distribution and for $\gamma \to 0$ it becomes the unitary distribution.[6]

If certain assumptions are made, the distribution of widths can be shown to be[7]

$$P_N(X, \gamma, \alpha) = \int \delta(X - NA_{11}^* A_{11}) p_N(H, \gamma, \alpha)\, dH_N, \tag{6}$$

where

$$X = \Gamma/\langle\Gamma\rangle, \tag{7}$$

Γ being the width and $\langle\Gamma\rangle$ the average width,

$$dH_N = \prod_{i>j} dR_{ij} \prod_{k>l} dS_{kl}, \tag{8}$$

and A is the unitary matrix which diagonalizes H, i.e.,

$$E = AHA^{\dagger} \tag{9}$$

where E is diagonal. It is the distribution $P_N(X, \gamma, \alpha)$ which we shall discuss in the remainder of this work.

* Supported in part by an N.R.C. grant.

[1] N. Rosenzweig, J. E. Monahan, and M. L. Mehta, Nucl. Phys. **A109**, 437 (1968). We refer to this paper as RMM.

[2] L. D. Favro and J. F. McDonald, Phys. Rev. Letters **19**, 1254 (1967).

[3] M. L. Mehta and N. Rosenzweig [Nucl. Phys. **A109**, 449 (1968)] obtained an analytical expression for the case when the invariant term is zero. However, this case is of no physical interest.

[4] A major difficulty seems to be a lack of a convenient parametrization for the rotation matrix.

[5] This distribution is the same as that used by RMM (except for a trivial scale change) if one takes $\gamma/\alpha = (1/\epsilon^2) - 2$.

[6] F. J. Dyson, J. Math. Phys. **3**, 140 (1962).

[7] See, for example, Ref. 1.

TABLE I. The values of A and C for various values of N and ϵ^2.

ϵ^2	N	10 $B=\frac{1}{3}$	20 $B=\frac{3}{20}$	30 $B=\frac{1}{9}$	50 $B=\frac{1}{15}$	100 $B=\frac{1}{30}$
0.001	A	0.50465 ± 0.00005	0.50865 ± 0.00005	0.51035 ± 0.00005	0.51515 ± 0.00005	0.52535 ± 0.00005
	C	6.7686 ± 0.0003	4.6616 ± 0.0003	4.1833 ± 0.0002	3.3108 ± 0.0002	2.4159 ± 0.0001
0.0025	A	0.51015 ± 0.00005	0.51795 ± 0.00005	0.52115 ± 0.00005	0.53045 ± 0.00005	0.54955 ± 0.00005
	C	4.3158 ± 0.0002	3.0002 ± 0.0002	2.7037 ± 0.0001	2.1635 ± 0.0001	1.6143 ± 0.0001
0.004	A	0.51475 ± 0.00005	0.52585 ± 0.00005	0.53025 ± 0.00005	0.54305 ± 0.00005	0.56885 ± 0.00005
	C	3.4353 ± 0.0002	2.4076 ± 0.0001	2.1770 ± 0.0001	1.7577 ± 0.0001	1.3348 ± 0.0001
0.0055	A	0.51905 ± 0.00005	0.53285 ± 0.00005	0.53835 ± 0.00005	0.55415 ± 0.00005	0.58545 ± 0.00005
	C	2.9481 ± 0.0001	2.0809 ± 0.0001	1.8873 ± 0.0001	1.5357 ± 0.0001	1.1837 ± 0.0001
0.007	A	0.52295 ± 0.00005	0.53935 ± 0.00005	0.54575 ± 0.00005	0.56405 ± 0.00005	0.60015 ± 0.00005
	C	2.6283 ± 0.0001	1.8675 ± 0.0001	1.6984 ± 0.0001	1.3915 ± 0.0001	1.0868 ± 0.0001
0.0085	A	0.52665 ± 0.00005	0.54535 ± 0.00005	0.55275 ± 0.00005	0.57345 ± 0.00005	0.61345 ± 0.00005
	C	2.3981 ± 0.0001	1.7144 ± 0.0001	1.5634 ± 0.0001	1.2891 ± 0.0001	1.0187 ± 0.0001
0.01	A	0.53025 ± 0.00005	0.55105 ± 0.00005	0.55925 ± 0.00005	0.58205 ± 0.00005	0.62555 ± 0.00005
	C	2.2225 ± 0.0001	1.5980 ± 0.0001	1.4607 ± 0.0001	1.2116 ± 0.0001	0.9677 ± 0.0001

3. THE SPECIAL CASE $N = 2$

For $N = 2$, the matrix A can be parametrized with the Cayley–Klein parameters.[2] When expressed in terms of the Eulerian angles (Goldstein's notation[8]) we have

$$A_{11} = A_{22}^* = e^{i(\psi+\phi)/2}\cos(\theta/2) \tag{10}$$

and

$$A_{12} = -A_{21}^* = ie^{i(\psi-\phi)/2}\sin(\theta/2). \tag{11}$$

It appears that there is an extra parameter here. However, the matrix elements H_{ij} are found to depend only on θ and ψ.

If the integration variables in (6) are changed from the R_{ij} and S_{ij} to the eigenvalues E_1 and E_2, and θ and ψ one obtains

$$\begin{aligned} P_2(X,\gamma,\alpha) = {} & [\alpha^{\frac{3}{2}}(\alpha+\gamma)^{\frac{1}{2}}/4\pi^2] \\ & \times \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 (E_1 - E_2)^2 \\ & \times \exp[-\alpha(E_1^2 + E_2^2)] \\ & \times \int_0^{2\pi} d\psi \int_0^{\pi} \sin\theta\, d\theta \\ & \times \exp\{-2\gamma[(E_1 - E_2)/2]^2 \sin^2\theta \cos^2\psi\} \\ & \times \delta[X - 2\cos^2(\theta/2)]. \end{aligned} \tag{12}$$

This expression can be reduced easily to

$$P_2(X,\gamma,\alpha) = (1+\beta)^{\frac{1}{2}} E[\beta\mu/(1+\beta\mu)]/\pi(1+\beta\mu)^{\frac{1}{2}}, \tag{13}$$

where

$$\beta = 2\gamma/\alpha, \tag{14}$$

$$\mu = X(1 - X/2), \tag{15}$$

and

$$E(m) = \int_0^{\pi/2} (1 - m\sin^2\theta)^{\frac{1}{2}}\, d\theta \tag{16}$$

is a complete elliptic integral of the second kind.[9]

4. CONJECTURE OF THE WIDTH DISTRIBUTION FOR ARBITRARY N

The limiting cases of $P_N(X, \gamma, \alpha)$ are[10]

$$\begin{aligned} P_N(X,\infty,\alpha) &= \frac{\Gamma(N/2)}{\Gamma((N-1)/2)} \frac{(1 - X/N)^{(N-3)/2}}{(\pi N X)^{\frac{1}{2}}} \\ &\xrightarrow[N\to\infty]{} \frac{e^{-x/2}}{(2\pi X)^{\frac{1}{2}}}, \end{aligned} \tag{17}$$

and[11]

$$P_N(X,0,\alpha) = \frac{N-1}{N}\left(1 - \frac{X}{N}\right)^{(N-2)} \xrightarrow[N\to\infty]{} e^{-X}. \tag{18}$$

Note that in each case the X dependence of P_N can be obtained from P_2 by replacing $(1 - X/2)$ with $(1 - X/N)$ and multiplying by $(1 - X/N)^{A(N-2)}$, where $A = \frac{1}{2}$ or 1 for the orthogonal or unitary case, respectively. We propose the same general procedure for the

[8] H. Goldstein, *Classical Mechanics* (Addison-Wesley Publ. Co., Inc., Reading, Mass., 1959), p. 109.

[9] *Applied Mathematics Series, No. 55: Handbook of Mathematical Functions* (National Bureau of Standards, Washington, D.C., 1964), p. 590.

[10] C. E. Porter and R. G. Thomas, Phys. Rev. **104**, 483 (1956).

[11] N. Ullah, J. Math. Phys. **4**, 1279 (1963).

general case. Thus, we surmise that

$$P_N(X, \gamma, \alpha) = C\{E[\beta\mu/(1 + \beta\mu)]/(1 + \beta\mu)^{\frac{1}{2}}\} \times (1 - X/N)^{A(N-2)}, \quad (19)$$

where now

$$\mu = X(1 - X/N) \quad (20)$$

and

$$\beta = B\gamma/\alpha. \quad (21)$$

For a given N and γ/α, there are three parameters A, B, and C which must be determined. However, there are only two conditions to be imposed on P_N. These are

$$\int_0^N X^n P_N(X, \gamma, \alpha)\, dX = 1, \quad n = 0, 1. \quad (22)$$

This means that some assumption about the parameters must be made. Our procedure will be to choose B and use (22) to obtain A and C.

5. COMPARISON WITH MONTE-CARLO CALCULATIONS

Rosenzweig, Monahan, and Mehta[1] have calculated the relative variance

$$R = \langle X^2 \rangle - 1, \quad (23)$$

for the ensemble given by (1), for $N = 10$, 20, 30, 50, and 100, with $0 \leq \epsilon^2 \leq 0.01$.[5] We found that we could choose a value of B for each N such that the values of R as calculated from (19) are approximately equal to their values for $0 \leq \epsilon^2 \leq 0.01$. That is, a B depending only on N and not ϵ^2. No attempt was made to choose a value of B such that our results best approximate theirs. Instead, for simplicity, B was chosen to be a rational number. The procedure then was to calculate A and C from (22) and use the results to calculate R.[12]

In Table I, we have given, for the values of B chosen, some selected values of A and C. In Fig. 1 we have given the results for R corresponding to these values of B. It can be seen that our results approximate those of RMM to within the error they give for $N = 10$, 20, 30, and 50 and $0 \leq \epsilon^2 \leq 0.01$. For $N = 100$, they are within the given error for $0 \leq \epsilon^2 \lesssim 0.0085$. However, for larger values of ϵ^2 our approximation is not as good. For example, at $\epsilon^2 = 0.01$ we disagree by about 3%. RMM also give a histogram for P_N with $N = 50$ and $\epsilon^2 = 0.01$. In Fig. 2 we have plotted the histogram corresponding to our P_N for these values. The two histograms appear to agree to within about 3%.

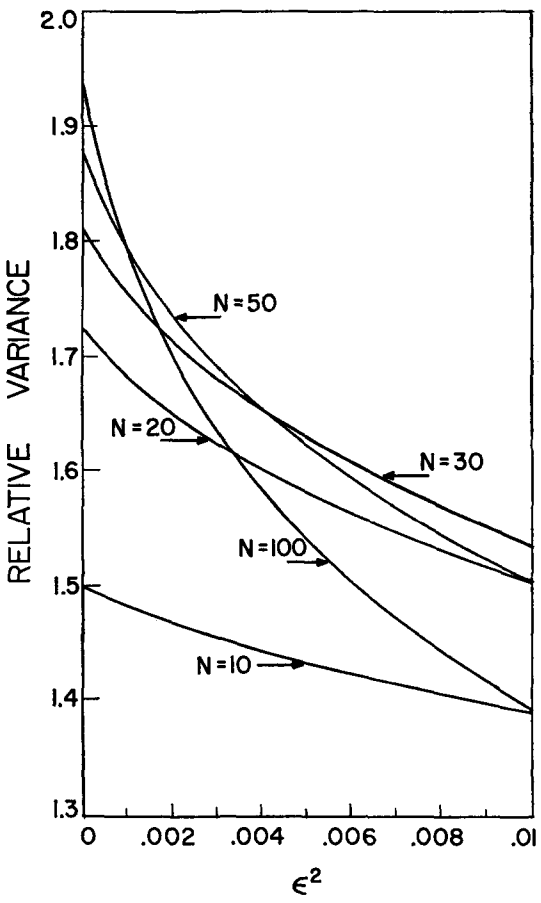

FIG. 1. Plot of the relative variance for $N = 10$, 20, 30, 50, 100.

Thus, based on a comparison with the limited numerical results available it appears that our distribution is a good approximation to the true distribution for large N and small ϵ^2. However, because of the apparent discrepancy for $N = 100$, $\epsilon^2 > 0.0085$, it is not clear that this approximation will continue to be valid for values of N much larger than 100 even for small values of ϵ^2.[13] That is, it may be that the region of validity will decrease in such a way that our expression is of little use in obtaining a limiting expression when $N \to \infty$. However, if it should turn out that it is valid for very large values of N and small but finite values of ϵ^2, there are some interesting consequences.

6. THE LIMIT OF OUR DISTRIBUTION AS $N \to \infty$

Note that the values of B chosen above are equal to $1/0.3N$ for $N = 30$, 50, and 100. Thus, it would appear that $B \propto 1/N$ for large N. The limit of our distribution depends on $\lim_{N\to\infty} B\gamma/\alpha$. Thus, there

[12] These calculations were carried out on the computer at the University of Windsor.

[13] This decrepancy could be removed by allowing B to depend on ϵ^2.

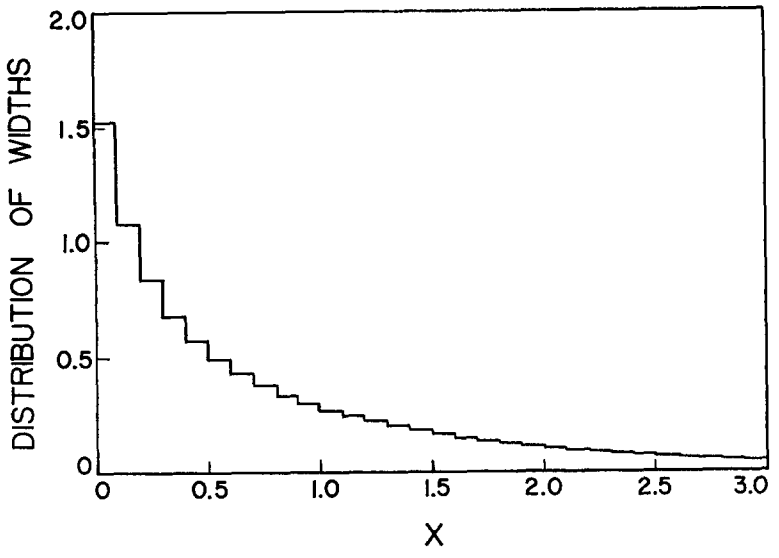

FIG. 2. Plot of histogram for $N = 50$, $\epsilon^2 = 0.01$.

appear to be three possibilities, namely,

(1) $\lim_{N\to\infty} P_N(X, \gamma, \alpha) \to e^{-X}$ (unitary),
if $\lim_{N\to\infty} B\gamma/\alpha \to 0$,

(2) $\lim_{N\to\infty} P_N(X, \gamma, \alpha) \to e^{-X/2}/(2\pi X)^{\frac{1}{2}}$ (orthogonal),
if $\lim_{N\to\infty} B\gamma/\alpha \to \infty$,

(3) $\lim_{N\to\infty} P_N(X, \gamma, \alpha) \to Ce^{-AX}/(1 + \tau X)^{\frac{1}{2}}$,
if $\lim_{N\to\infty} B\gamma/\alpha \to \tau$, where $\tau > 0$ and finite.

If γ/α is independent of N, the distribution is the orthogonal result at $\epsilon^2 = 0$ and the unitary result for all $\epsilon^2 \neq 0$. Only if $\epsilon^2 \propto 1/N$ is an intermediate limiting form obtained. This in effect says that there is no such thing as a small but finite noninvariant perturbation.

This last conclusion seems unrealistic from a physical point of view. The effect may simply be a result of the ensemble assumed. That is, perhaps there are too many matrix elements S_{ij} which are nonzero simultaneously for this ensemble. The same type of thing occurs in an ordinary perturbation expansion for the eigenvalues and eigenvectors for a fixed Hamiltonian if too many matrix elements are nonzero.

Thus, it appears that one must do one of four things:

(1) Require that $\epsilon^2 \propto 1/N$,

(2) give up the Gaussian ensemble,

(3) use a Gaussian ensemble, but somehow restrict it so that only a finite number of the S_{ij} can be nonzero simultaneously,

(4) not take the limit as $N \to \infty$, but rather give a more precise meaning to N.

The second alternative seems undesirable in view of the success of the Gaussian distribution in the limiting cases.[14] The third alternative is perhaps a special case of the fourth, which has been previously suggested.[1] Also, it seems that the first alternative might just be one way of accomplishing the third.

It should be remembered, of course, that the conclusions of this section are based on a hypothesis which has not been rigorously proven. That is, we have assumed that our expression for P_N is meaningful for $N \to \infty$.

[14] See, for example, *Statistical Theories of Spectra: Fluctuations*, C. E. Porter, Ed. (Academic Press Inc., New York, 1965). Most of the pertinent papers (including Refs. 6, 9, and 10 above) are contained in this collection, as well as an excellent introductory review of this subject. See also M. L. Mehta, *Random Matrices and the Statistical Theory of Energy Levels* (Academic Press Inc., New York, 1967).

Type D Vacuum Metrics*

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(Received 17 May 1968)

Using the Newman–Penrose formalism, the vacuum field equations are solved for Petrov type D. An exhaustive set of ten metrics is obtained, including among them a new rotating solution closely related to the Ehlers–Kundt "C" metric. They all possess at least two Killing vectors and depend only on a small number of arbitrary constants.

1. INTRODUCTION

It was once supposed that algebraically special fields would play a central role in the search for an exact gravitational-wave solution radiating from a finite source. Now we know such solutions must unfortunately be Petrov type I. Since it seems a large step up to the greatest generality of type I gravitational fields, perhaps it is appropriate at this stage to return to the algebraically special cases and make sure that they are thoroughly understood despite their limitations.

Petrov type D is a particularly interesting class to study for several reasons. The Schwarzschild and Kerr[1] metrics are familiar members of this class. Besides being free of the line singularities which plague most algebraically special metrics,[2] these two metrics are also stationary in time. Do all type D fields share this property? The relation between Petrov type and the existence of Killing vectors is not known; but at least one can easily prove a weak converse, namely that an algebraically special field which is stationary, time reversible, and with a finite source can only be type D.[3]

In this paper we will derive all type D vacuum metrics. The line of attack will be the Newman–Penrose (NP) tetrad formalism[4] which has proved its usefulness in many related investigations.[5,6] For those unfamiliar with the formalism and not wishing to take the time to learn it, the final metrics are written out in full at the end of each section.

2. NP EQUATIONS

Let the space be vacuum and type D. Let l^μ, n^μ, m^μ, $\bar{m}^\mu$ be a quasiorthonormal tetrad and choose l^μ and n^μ to lie along the principal null directions. In the notation of Ref. 4 this implies $\psi_0 = \psi_1 = \psi_3 = \psi_4 = 0$. We will refer to ψ_2 as just ψ from now on for convenience. The Goldberg–Sachs theorem implies $\kappa = \sigma = \nu = \lambda = 0$. As usual, we choose coordinates such that $l^\mu = \delta^\mu_2$, making $x^2 = r$ an affine parameter along l^μ, and we set $\epsilon = 0$. The tetrad components are

$$\begin{aligned} l^\mu &= (0, 1, 0, 0), \\ n^\mu &= (X^1, U, X^3, X^4), \\ m^\mu &= (\xi^1, \omega, \xi^3, \xi^4). \end{aligned} \tag{2.1}$$

The NP equations under these assumptions are

$$DU = (\bar{\tau} + \pi)\omega + (\tau + \bar{\pi})\bar{\omega} - (\gamma + \bar{\gamma}), \tag{2.2a}$$
$$DX^i = (\bar{\tau} + \pi)\xi^i + (\tau + \bar{\pi})\bar{\xi}^i, \tag{2.2b}$$
$$D\omega = \bar{\rho}\omega + (\bar{\pi} - \bar{\alpha} - \beta), \tag{2.2c}$$
$$D\xi^i = \bar{\rho}\xi^i, \tag{2.2d}$$
$$\begin{aligned} \delta U - \Delta\omega = {} & (\tau - \bar{\alpha} - \beta)U \\ & + (\mu - \gamma + \bar{\gamma})\omega, \end{aligned} \tag{2.3a}$$
$$\begin{aligned} \delta X^i - \Delta\xi^i = {} & (\tau - \bar{\alpha} - \beta)X^i \\ & + (\mu - \gamma + \bar{\gamma})\xi^i, \end{aligned} \tag{2.3b}$$
$$\begin{aligned} \bar{\delta}\omega - \delta\bar{\omega} = {} & (\bar{\mu} - \mu) + (\bar{\rho} - \rho)U \\ & - (\bar{\beta} - \alpha)\omega - (\bar{\alpha} - \beta)\bar{\omega}, \end{aligned} \tag{2.3c}$$
$$\begin{aligned} \bar{\delta}\xi^i - \delta\bar{\xi}^i = {} & (\bar{\rho} - \rho)X^i - (\bar{\beta} - \alpha)\xi^i \\ & - (\bar{\alpha} - \beta)\bar{\xi}^i, \end{aligned} \tag{2.3d}$$
$$D\rho = \rho^2, \tag{2.4a}$$
$$D\beta = \bar{\rho}\beta, \tag{2.4b}$$
$$D\alpha = \rho(\alpha + \pi), \tag{2.4c}$$
$$D\tau = \rho(\tau + \bar{\pi}), \tag{2.4d}$$
$$D\gamma = \alpha(\tau + \bar{\pi}) + \beta(\bar{\tau} + \pi) + \tau\pi + \psi, \tag{2.4e}$$
$$D\mu - \delta\pi = \bar{\rho}\mu + \pi(\bar{\pi} - \bar{\alpha} + \beta) + \psi, \tag{2.4f}$$

* Supported in part by the National Science Foundation [GP-7976, formerly GP-5391] and the Office of Naval Research [Nonr-220(47)].

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[1] R. Kerr, Phys. Rev. Letters **11**, 522 (1963).

[2] I. Robinson and A. Trautman, Proc. Roy. Soc. (London) **265**, 463 (1962).

[3] "Stationary and time-reversible" implies that at any point there exists an isometry which leaves the point fixed and interchanges the light cones. Any isometry must also map the null congruences into themselves. Since the expansion of the congruences is nonzero for a finite source, the "outward" sense on each congruence is uniquely specified, and preserved under isometries. Then any double null vector and its time-reversed image must be distinct.

[4] E. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).

[5] E. Newman, L. Tamburino, and T. Unti, J. Math. Phys. **4**, 915 (1963).

[6] E. Newman and L. Tamburino, J. Math. Phys. **3**, 902 (1962).

$$\delta\rho = \rho(\bar{\alpha} + \beta) + (\rho - \bar{\rho})\tau, \tag{2.5a}$$

$$\delta\tau = \tau(\tau - \bar{\alpha} + \beta), \tag{2.5b}$$

$$\delta\alpha - \bar{\delta}\beta = \rho\mu + \alpha\bar{\alpha} + \beta\bar{\beta} - 2\alpha\beta + (\rho - \bar{\rho})\gamma - \psi, \tag{2.5c}$$

$$\bar{\delta}\pi = -\pi(\pi + \alpha - \bar{\beta}), \tag{2.5d}$$

$$\bar{\delta}\mu = -\mu(\alpha + \bar{\beta}) - (\mu - \bar{\mu})\pi, \tag{2.5e}$$

$$\Delta\rho - \bar{\delta}\tau = -\rho\bar{\mu} - \tau(\bar{\tau} + \alpha - \bar{\beta}) + \rho(\gamma + \bar{\gamma}) - \psi, \tag{2.6a}$$

$$\Delta\pi = -\mu(\bar{\tau} + \pi) - \pi(\gamma - \bar{\gamma}), \tag{2.6b}$$

$$\Delta\alpha - \bar{\delta}\gamma = -\bar{\mu}\alpha + \gamma(\bar{\beta} - \bar{\tau}) + \bar{\gamma}\alpha, \tag{2.6c}$$

$$\Delta\beta - \delta\gamma = -\mu(\beta + \tau) + \gamma(2\beta + \bar{\alpha} - \tau) - \bar{\gamma}\beta, \tag{2.6d}$$

$$\Delta\mu = -\mu(\mu + \gamma + \bar{\gamma}). \tag{2.6e}$$

The Bianchi identities are

$$D\psi = 3\rho\psi, \tag{2.7a}$$

$$\Delta\psi = -3\mu\psi, \tag{2.7b}$$

$$\delta\psi = 3\tau\psi, \tag{2.7c}$$

$$\bar{\delta}\psi = -3\pi\psi, \tag{2.7d}$$

and the commutation relations are

$$\begin{aligned}
\Delta D - D\Delta &= (\gamma + \bar{\gamma})D - (\bar{\tau} + \pi)\delta \\
&\quad - (\tau + \bar{\pi})\bar{\delta}, \\
\delta D - D\delta &= (\bar{\alpha} + \beta - \pi)D - \bar{\rho}\delta, \\
\delta\Delta - \Delta\delta &= (\tau - \bar{\alpha} - \beta)D \\
&\quad + (\mu - \gamma + \bar{\gamma})\delta, \\
\bar{\delta}\delta - \delta\bar{\delta} &= (\bar{\mu} - \mu)D + (\bar{\rho} - \rho)\Delta \\
&\quad - (\bar{\beta} - \alpha)\delta - (\bar{\alpha} - \beta)\bar{\delta}.
\end{aligned} \tag{2.8}$$

In addition to the above equations we get three more important relations among the tetrad variables by applying the commutators to ψ:

$$\begin{aligned}
(\Delta D - D\Delta)\psi &= \Delta(3\rho\psi) - D(-3\mu\psi) \\
&= 3\psi(\Delta\rho + D\mu) \\
&= 3\psi[\rho(\gamma + \bar{\gamma}) - \tau(\bar{\tau} + \pi) \\
&\quad + \pi(\tau + \bar{\pi})] \\
\Rightarrow \Delta\rho + D\mu &= \rho(\gamma + \bar{\gamma}) + \pi\bar{\pi} - \tau\bar{\tau}.
\end{aligned} \tag{2.9}$$

Likewise from $(\bar{\delta}D - D\bar{\delta})\psi$ and $(\delta\Delta - \Delta\delta)\psi$ we get

$$\bar{\delta}\rho + D\pi = \rho(\alpha + \bar{\beta}), \tag{2.10}$$

$$\delta\mu + \Delta\tau = -\mu(\bar{\alpha} + \beta) + \tau(\gamma - \bar{\gamma}). \tag{2.11}$$

The other commutators give no new information.

The integration of the NP equations falls naturally into two cases to consider, $\rho \neq 0$ and $\rho = 0$.

3. SOLUTION FOR $\rho \neq 0$

A. Radial Integration

The solution to $D\rho = \rho^2$, Eq. (2.4a), is

$$\rho = -(r + i\rho^0)^{-1}, \tag{3.1}$$

where ρ^0 is real and the superscript indicates it is independent of r. The case $\rho = 0$, resulting from $\rho^0 \to \infty$, will be considered separately later.

An equation for $\bar{\delta}\rho$ may be derived from the commutator

$$\begin{aligned}
(\bar{\delta}D - D\bar{\delta})\rho &= 2\rho\bar{\delta}\rho - D\bar{\delta}\rho \\
&= \rho^2(\alpha + \bar{\beta} - \pi) - \rho\bar{\delta}\rho,
\end{aligned}$$

giving

$$D\bar{\delta}\rho - 3\rho\bar{\delta}\rho = \rho^2(\pi - \alpha - \bar{\beta}). \tag{3.2}$$

Using Eqs. (2.4a)–(2.4c), the general solution of this is found to be

$$\bar{\delta}\rho = \rho(\alpha + \bar{\beta}) - 2\bar{\tau}^0\rho^3, \tag{3.3}$$

where $\bar{\tau}^0$ is a "constant" of integration, i.e., independent of r. This result is substituted in Eq. (2.10) to get

$$D\pi = 2\bar{\tau}^0\rho^3, \tag{3.4}$$

which has the solution

$$\pi = \pi^0 + \bar{\tau}^0\rho^2. \tag{3.5}$$

Equations (2.2), (2.4b)–(2.4e), and (2.7a) now can be integrated easily one at a time, each one yielding a new integration constant. In this way the radial dependence of every tetrad variable except μ is determined; the solutions are as follows:

$$\beta = \bar{\rho}\beta^0, \tag{3.6a}$$

$$\alpha = \rho\alpha^0 - \pi^0 + \rho^2\bar{\tau}^0, \tag{3.6b}$$

$$\tau = \rho\eta^0 + \rho\bar{\rho}\tau^0 - \bar{\pi}^0, \tag{3.6c}$$

$$\omega = \bar{\rho}\omega^0 + \bar{\alpha}^0 + \beta^0 - \bar{\pi}^0/\bar{\rho}, \tag{3.6d}$$

$$\xi^i = \bar{\rho}\xi^{0i}, \tag{3.6e}$$

$$\begin{aligned}
X^i = X^{0i} &+ \rho\bar{\rho}(\bar{\tau}^0\xi^{0i} + \tau^0\bar{\xi}^{0i}) + \rho\eta^0\bar{\xi}^{0i} \\
&+ \bar{\rho}\bar{\eta}^0\xi^{0i},
\end{aligned} \tag{3.6f}$$

$$\psi = \rho^3\psi^0, \tag{3.6g}$$

$$\begin{aligned}
\gamma = \gamma^0 &+ \rho(\eta^0\alpha^0 - \bar{\tau}^0\bar{\pi}^0) + \bar{\rho}(\bar{\eta}^0\beta^0 - \tau^0\pi^0) \\
&+ \rho^2(\tfrac{1}{2}\psi^0 + \bar{\tau}^0\eta^0) + \rho\bar{\rho}(\tau^0\alpha^0 + \bar{\tau}^0\beta^0) \\
&+ \rho^2\bar{\rho}\tau^0\bar{\tau}^0 - r\pi^0\bar{\pi}^0,
\end{aligned} \tag{3.6h}$$

$$\begin{aligned}
U = U^0 &- r(\gamma^0 + \bar{\gamma}^0 + \eta^0\pi^0 + \bar{\eta}^0\bar{\pi}^0) + r^2\pi^0\bar{\pi}^0 \\
&+ \rho[\bar{\tau}^0(\bar{\alpha}^0 + \beta^0) - \bar{\tau}^0\eta^0 + \eta^0\bar{\omega}^0 - \tfrac{1}{2}\psi^0] \\
&+ \bar{\rho}[\tau^0(\alpha^0 + \beta^0) - \tau^0\bar{\eta}^0 + \bar{\eta}^0\omega^0 - \tfrac{1}{2}\bar{\psi}^0] \\
&+ \rho\bar{\rho}(\bar{\tau}^0\omega^0 + \tau^0\bar{\omega}^0 - \tau^0\bar{\tau}^0) - (\rho/\bar{\rho})\bar{\tau}^0\bar{\pi}^0 \\
&- (\bar{\rho}/\rho)\tau^0\pi^0.
\end{aligned} \tag{3.6i}$$

To get an expression for $\Delta\rho$ and μ we again need to use a commutator:

$$\begin{aligned}(\Delta D - D\Delta)\rho &= 2\rho\Delta\rho - D\Delta\rho \\ &= \rho^2(\gamma + \bar{\gamma}) - (\tau + \bar{\pi})\delta\rho \\ &\quad - (\bar{\tau} + \pi)\delta\rho.\end{aligned}$$

The last member of this equation can be written out in full using Eqs. (2.5a), (3.3), (3.5), and (3.6). The result is an equation for $\Delta\rho$, which can be integrated to give

$$\begin{aligned}\Delta\rho = &-\rho^2 M^0 + \rho^2\eta^0(\alpha^0 + \bar{\beta}^0) \\ &+ \rho(\gamma^0 + \bar{\gamma}^0 + \eta^0\pi^0) + \bar{\rho}^0\bar{\eta}^0\bar{\pi}^0 \\ &+ \rho\bar{\rho}[\bar{\eta}^0(\bar{\alpha}^0 + \beta^0) - \tau^0\pi^0 + \bar{\tau}^0\bar{\pi}^0 - \eta^0\bar{\eta}^0] \\ &- \rho^3(\tfrac{1}{2}\psi^0 + \bar{\tau}^0\eta^0) - \rho^2\bar{\rho}[\tfrac{1}{2}\bar{\psi}^0 + \bar{\tau}^0\eta^0 \\ &- \tau^0(\alpha^0 + \bar{\beta}^0) - \bar{\tau}^0(\bar{\alpha}^0 + \beta^0)] \\ &- \rho^3\bar{\rho}\tau^0\bar{\tau}^0 + r^2\rho^2\pi^0\bar{\pi}^0, \qquad (3.7)\end{aligned}$$

where M^0 is the constant of integration. Finally we substitute this into Eq. (2.9) and perform the radial integration for μ, getting

$$\begin{aligned}\mu = &\mu^0 + \rho(M^0 - \bar{\tau}^0\bar{\pi}^0) + \bar{\rho}\tau^0\pi^0 \\ &+ \rho^2(\tfrac{1}{2}\psi^0 + \bar{\tau}^0\eta^0) + \tfrac{1}{2}\rho\bar{\rho}\bar{\psi}^0 \\ &+ \rho^2\bar{\rho}\tau^0\bar{\tau}^0 - r^2\rho\pi^0\bar{\pi}^0. \qquad (3.8)\end{aligned}$$

B. Transverse Equations

In the second stage of the solution we complete the elimination of r by substituting these results into the remaining equations and equating the coefficients of like powers of ρ. In this manner we obtain differential equations involving ξ^{0i} and X^{0i}, and also some purely algebraic constraints between the integration constants.

To find the derivatives of ρ^0 we differentiate Eq. (3.1):

$$\begin{aligned}\delta\rho &= \rho^2(\omega + i\delta\rho^0), \\ \bar{\delta}\rho &= \rho^2(\bar{\omega} + i\bar{\delta}\rho^0), \\ \Delta\rho &= \rho^2(U + i\Delta\rho^0).\end{aligned}$$

When these are expanded and compared with Eqs. (2.5a), (3.3), and (3.7),we get the following information:

$$\xi^{0i}\rho^0_{,i} = -\rho^0(\bar{\alpha}^0 + \beta^0 - \eta^0) - i\tau^0 + 2i(\rho^0)^2\bar{\pi}^0, \qquad (3.9)$$

$$\begin{aligned}X^{0i}\rho^0_{,i} = &-\rho^0(\gamma^0 + \bar{\gamma}^0 + 2\pi^0\eta^0 + 2\bar{\pi}^0\bar{\eta}^0) \\ &+ \tfrac{1}{2}i(M^0 - \bar{M}^0) + i(\tau^0\pi^0 - \bar{\tau}^0\bar{\pi}^0), \qquad (3.10)\end{aligned}$$

$$\omega^0 = -i\rho^0(\bar{\alpha}^0 + \beta^0 - \eta^0) - 2(\rho^0)^2\bar{\pi}^0, \qquad (3.11)$$

$$\begin{aligned}U^0 = &\eta^0(\alpha^0 + \bar{\beta}^0) + \bar{\eta}^0(\bar{\alpha}^0 + \beta^0) - \eta^0\bar{\eta}^0 \\ &+ i\rho^0(\pi^0\eta^0 - \bar{\pi}^0\bar{\eta}^0) - \tfrac{1}{2}(M^0 + \bar{M}^0) \\ &+ \tau^0\pi^0 + \bar{\tau}^0\bar{\pi}^0. \qquad (3.12)\end{aligned}$$

The three other Bianchi identities, Eqs. (2.7b)–(2.7d), provide the derivatives of ψ^0:

$$\xi^{0i}\psi^0_{,i} = -3\psi^0(\bar{\alpha}^0 + \beta^0 - \eta^0 - 2i\rho^0\bar{\pi}^0), \qquad (3.13)$$

$$\bar{\xi}^{0i}\psi^0_{,i} = -3\psi^0(\alpha^0 + \bar{\beta}^0), \qquad (3.14)$$

$$X^{0i}\psi^0_{,i} = -3\psi^0(\gamma^0 + \bar{\gamma}^0 + \mu^0 + \pi^0\eta^0 + \bar{\pi}^0\bar{\eta}^0). \qquad (3.15)$$

Substitution in Eqs. (2.5b) and (2.6a) gives the transverse derivatives of π^0, τ^0, η^0:

$$\xi^{0i}\pi^0_{,i} = -\mu^0 + \pi^0(\bar{\alpha}^0 - \beta^0), \qquad (3.16)$$

$$\bar{\xi}^{0i}\pi^0_{,i} = \pi^0(\bar{\beta}^0 - \alpha^0), \qquad (3.17)$$

$$\xi^{0i}\tau^0_{,i} = -\tau^0(3\bar{\alpha}^0 + \beta^0), \qquad (3.18)$$

$$\begin{aligned}\bar{\xi}^{0i}\tau^0_{,i} = &-\tau^0(\alpha^0 + 3\bar{\beta}^0 - \bar{\eta}^0 + 2i\rho^0\pi^0) - 2i\rho^0\bar{M}^0 \\ &- 2i(\rho^0)^3\pi^0\bar{\pi}^0 + \tfrac{1}{2}(\psi^0 - \bar{\psi}^0), \qquad (3.19)\end{aligned}$$

$$\xi^{0i}\eta^0_{,i} = -\eta^0(2\bar{\alpha}^0 - \eta^0 - 2i\rho^0\bar{\pi}^0) + 2\tau^0\bar{\pi}^0, \qquad (3.20)$$

$$\bar{\xi}^{0i}\eta^0_{,i} = -2\bar{\beta}^0\eta^0 - M^0 + \bar{M}^0 + 2\bar{\tau}^0\bar{\pi}^0. \qquad (3.21)$$

Equations (2.4f) and (2.5d) merely confirm these results. Equation (2.5c) yields

$$\begin{aligned}\xi^{0i}\alpha^0_{,i} - \bar{\xi}^{0i}\beta^0_{,i} = &2\beta^0(\bar{\beta}^0 - \alpha^0) \\ &+ 2i\rho^0(\gamma^0 + \mu^0 + \alpha^0\bar{\pi}^0 + \beta^0\pi^0) \\ &+ M^0 + 3(\rho^0)^2\pi^0\bar{\pi}^0. \qquad (3.22)\end{aligned}$$

Equation (2.5e) yields the derivatives

$$\begin{aligned}\bar{\xi}^{0i}\mu^0_{,i} = &-\mu^0(\alpha^0 + \bar{\beta}^0) - 2i\rho^0\bar{\mu}^0\pi^0 + 2i\rho^0\pi^0\bar{\pi}^0\bar{\eta}^0 \\ &+ (M^0 + \bar{M}^0)\pi^0 + 6(\rho^0)^2\pi^0\pi^0\bar{\pi}^0, \qquad (3.23)\end{aligned}$$

$$\begin{aligned}\bar{\xi}^{0i}M^0_{,i} = &-2M^0(\alpha^0 + \bar{\beta}^0) + (\psi^0 + 2\bar{\psi}^0)\pi^0 + (\rho^0)^2\bar{\mu}^0\pi^0 \\ &- 2\mu^0\bar{\tau}^0 + 2\bar{\tau}^0\pi^0\eta^0 - 2(\rho^0)^2\pi^0\bar{\pi}^0\bar{\eta}^0 \\ &+ 2i\rho^0\bar{\tau}^0\bar{\pi}^0\pi^0 + 4i(\rho^0)^3\pi^0\pi^0\bar{\pi}^0, \qquad (3.24)\end{aligned}$$

and a very important relation

$$\eta^0 = 2i\rho^0\bar{\pi}^0. \qquad (3.25)$$

When this last constraint is introduced, many of the above equations simplify. If we differentiate it and compare with Eq. (3.21) we get another condition

$$M^0 - \bar{M}^0 = 2i\rho^0\bar{\mu}^0 + 4\bar{\tau}^0\bar{\pi}^0 - 8(\rho^0)^2\pi^0\bar{\pi}^0; \qquad (3.26)$$

and since the real part of the right-hand side must vanish, we have also

$$2\tau^0\pi^0 + 2\bar{\tau}^0\bar{\pi}^0 = 8(\rho^0)^2\pi^0\bar{\pi}^0 + i\rho^0(\mu^0 - \bar{\mu}^0). \qquad (3.27)$$

Continuing in the same manner, Eqs. (2.6) and (2.11)

give

$$\xi^{0i}\mu^0_{,i} = -\mu^0(\bar\alpha^0 + \beta^0) + \bar\pi^0(M^0 + \bar M^0) + 2i\rho^0\bar\pi^0\mu^0 + 10(\rho^0)^2\pi^0\bar\pi^0\bar\pi^0, \tag{3.28}$$

$$\xi^{0i}M^0_{,i} = -2M^0(\bar\alpha^0 + \beta^0) + 3\bar\pi^0\bar\psi^0 + 2i\rho^0\bar\pi^0(5M^0 + \bar M^0) - 3(\rho^0)^2\mu^0\bar\pi^0 - 6i\rho^0\tau^0\pi^0\bar\pi^0 + 20i(\rho^0)^3\pi^0\bar\pi^0\bar\pi^0, \tag{3.29}$$

$$X^{0i}\pi^0_{,i} = -\pi^0(\gamma^0 - \bar\gamma^0 + 2i\rho^0\pi^0\bar\pi^0), \tag{3.30}$$

$$X^{0i}\tau^0_{,i} = -\tau^0(\mu^0 + \gamma^0 + 3\bar\gamma^0) + \tfrac{1}{2}\bar\pi^0(\psi - \bar\psi^0) - 2i\rho^0\bar\pi^0M^0 + 6i\rho^0\tau^0\pi^0\pi^0 - 2i(\rho^0)^3\pi^0\bar\pi^0\bar\pi^0, \tag{3.31}$$

$$X^{0i}\alpha^0_{,i} - \xi^{0i}\gamma^0_{,i} = -\alpha^0(\bar\mu^0 + \gamma^0) + \bar\beta^0\gamma^0 + i\rho^0\pi^0(2\gamma^0 + 2\mu^0 - \bar\mu^0) + \bar M^0\pi^0 + 2i\rho^0\pi^0\pi^0\beta^0 - 4i\rho^0\pi^0\bar\pi^0\alpha^0 + \bar\tau^0\bar\pi^0\pi^0 + 7(\rho^0)^2\pi^0\pi^0\bar\pi^0, \tag{3.32}$$

$$X^{0i}\beta^0_{,i} - \xi^{0i}\gamma^0_{,i} = -\beta^0(\mu^0 - \gamma^0 + 2\bar\gamma^0) + \bar\alpha^0\gamma^0 - i\rho^0\bar\pi^0(2\gamma^0 + \mu^0) + M^0\bar\pi^0 + 4i\rho^0\pi^0\bar\pi^0\beta^0 - 2i\rho^0\bar\pi^0\bar\pi^0\alpha^0 + 3\tau^0\pi^0\bar\pi^0 + 3(\rho^0)^2\pi^0\bar\pi^0\bar\pi^0, \tag{3.33}$$

$$X^{0i}\mu^0_{,i} = -\mu^0(\mu^0 + \gamma^0 + \bar\gamma^0 - 2i\rho^0\pi^0\bar\pi^0) - 2i\rho^0\pi^0\bar\pi^0\bar\mu^0, \tag{3.34}$$

$$X^{0i}M^0_{,i} = -2M^0(\mu^0 + \gamma^0 + \bar\gamma^0) - \pi^0\bar\pi^0(\psi^0 - \bar\psi^0) + 4i\rho^0M^0\pi^0\bar\pi^0 + 2\mu^0\bar\tau^0\bar\pi^0 + (\rho^0)^2\pi^0\bar\pi^0 \times (\mu^0 - \bar\mu^0) + 4i\rho^0\bar\pi^0\pi^0\pi^0\tau^0 - 4i\rho^0\bar\pi^0\bar\pi^0\pi^0\tau^0 - 12i(\rho^0)^3\pi^0\pi^0\bar\pi^0\bar\pi^0, \tag{3.35}$$

and an algebraic constraint

$$\mu^0 = \bar\mu^0. \tag{3.36}$$

It is interesting to note that this constraint is implied only by the very last equation, Eq. (2.6e). Differentiation of Eq. (3.27) leads to

$$\tfrac{1}{2}\pi^0(\psi^0 - \bar\psi^0) = -\mu^0\tau^0 + 4(\rho^0)^2\mu^0\bar\pi^0 + 2i\rho^0M^0\bar\pi^0 + 2i\rho^0\tau^0\pi^0\bar\pi^0 - 2i\rho^0\bar\tau^0\bar\pi^0\pi^0 - 6i(\rho^0)^3\pi^0\bar\pi^0\bar\pi^0. \tag{3.37}$$

Finally, the metric equations (2.3) give

$$\xi^{0i}X^{0j}_{,i} - X^{0i}\xi^{0j}_{,i} = (\mu^0 + 2\bar\gamma^0 - 4i\rho^0\bar\pi^0\pi^0)\xi^{0j} + 2i\rho^0\pi^0\bar\pi^0\bar\xi^{0j} + (2i\rho^0\bar\pi^0 - \bar\alpha^0 - \beta^0)X^{0j}, \tag{3.38}$$

$$\bar\xi^{0i}\xi^{0j}_{,i} - \xi^{0i}\bar\xi^{0j}_{,i} = (-2\bar\beta^0 - 2i\rho^0\pi^0)\xi^{0j} + (2\beta^0 - 2i\rho^0\bar\pi^0)\bar\xi^{0j} - 2i\rho^0X^{0j}. \tag{3.39}$$

The lengthy algebra involved in this section has been verified using a FORMAC computer program.

C. Choice of Tetrad and Coordinates

So far the tetrad is not completely specified; it has the freedom of the two-parameter group of rotations which leaves the directions of l^μ and n^μ fixed:

$$l^\mu \to (A^0)^{-1}l^\mu, \quad n^\mu \to A^0n^\mu, \quad m^\mu \to m^\mu\exp(i\theta^0), \tag{3.40}$$

where A^0 and θ^0 are arbitrary real functions independent of r. (If they were allowed to depend on r, the condition $\epsilon = 0$ would be violated.) This group induces a transformation on all the tetrad variables. For instance,

$$\begin{aligned} U^0 &\to (A^0)^2U^0, \\ \psi^0 &\to (A^0)^3\psi^0, \\ \alpha^0 + \bar\beta^0 &\to [A^0(\alpha^0 + \bar\beta^0) - \bar\xi^{0j}A^0_{,j}]\exp(i\theta^0), \\ \pi^0 &\to \pi^0\exp(-i\theta^0), \\ \tau^0 &\to (A^0)^2\tau^0\exp(i\theta^0). \end{aligned} \tag{3.41}$$

The fact that some variables transform inhomogeneously permits a partial check on the results of Sec. 3B, since all the equations obtained there must be covariant under the group. It also raises the possibility of setting some of the variables to zero.

We perform a rotation with A^0 chosen such that $\psi^0\bar\psi^0$ becomes a constant. Then Eqs. (3.13)–(3.15) tell us that

$$\bar\alpha^0 + \beta^0 = 2i\rho^0\bar\pi^0, \tag{3.42}$$

$$\gamma^0 + \bar\gamma^0 + \mu^0 = 0. \tag{3.43}$$

At this point it is necessary to resolve several cases.

Case I: $\pi^0 = \tau^0 = 0$. This is the case already treated in Ref. 5 and leads to the three NUT metrics.

Case II: $\pi^0 = 0$, $\tau^0 \neq 0$. We select θ^0 such that $i\tau^0$ is everywhere real and positive. Equations (3.16), (3.31), and (3.43) tell us $\mu^0 = \gamma^0 = 0$. Now $M^0 = -U^0$ and $\psi^0 \equiv m + il$ become constants. From a comparison of Eqs. (3.18), (3.19), and (3.22) we get

$$\begin{aligned} \beta^0 &= \bar\beta^0, \\ 2\rho^0U^0 &= -l - 4i\beta^0\tau^0, \\ \xi^{0i}\beta^0_{,i} &= \tfrac{1}{2}U^0 - 2(\beta^0)^2, \\ \xi^{0i}\tau^0_{,i} &= 2\beta^0\tau^0. \end{aligned} \tag{3.44}$$

Choose coordinates such that $X^{0i} = \delta_{i1}$. Use $\rho^0 \neq$ const to define a coordinate x^3 by $\rho^0 = \rho^0(x^3)$. As $\xi^{0i}\rho^0_{,i}$ is real, so ξ^{03} must also be real. By coordinate transformations

$$x^1 \to x^1 + f(x^3, x^4), \quad x^3 \to g(x^3), \quad x^4 \to x^4 + h(x^3, x^4) \tag{3.45}$$

make $\xi^{03} = -(2)^{-\frac{1}{2}}$ and ξ^{01}, ξ^{04} imaginary. Then,

$$\xi^{0i}\xi^{0j}_{,i} = \bar{\xi}^{0i}\xi^{0j}_{i},$$
$$\xi^{0i}\tau^{0}_{,i} = \bar{\xi}^{0i}\tau^{0}_{,i},$$
$$\xi^{0i}\beta^{0}_{,i} = \bar{\xi}^{0i}\beta^{0}_{i},$$
$$X^{0i}\xi^{0j}_{,i} = X^{0i}\tau^{0}_{,i} = X^{0i}\beta^{0}_{,i} = 0$$

show that ξ^{0i}, τ^0, β^0 are functions of only one coordinate, x^3. Integration is straightforward and leads to the following metrics:

Case II.A: $U^0 < 0$. By a further rotation [Eq. (3.40)] with A^0 constant, set $U^0 = -\frac{1}{2}$. The solution is Kerr–NUT space[7] with a the Kerr parameter and $x^1 = u$, $x^2 = r$, $x^3 = x$, $x^4 = y$:

$$\begin{aligned}
\beta^0 &= -\tfrac{1}{4}(2)^{\frac{1}{2}}\cot x,\\
\tau^0 &= -\tfrac{1}{2}ia(2)^{\frac{1}{2}}\sin x,\\
\rho &= -(r + il - ia\cos x)^{-1},\\
l^\mu &= (0, 1, 0, 0),\\
n^\mu &= \rho\bar{\rho}[r^2 + l^2 + a^2, -\tfrac{1}{2}(r^2 - 2mr - l^2 + a^2), 0, a],\\
m^\mu &= -\tfrac{1}{2}(2)^{\frac{1}{2}}\bar{\rho}[ia\sin x + 2il\cot x, 0, 1, i\csc x].
\end{aligned} \tag{3.46}$$

The only nonzero components of the metric are

$$\begin{aligned}
g_{uu} &= \rho\bar{\rho}(r^2 - 2mr - l^2 + a^2\cos^2 x),\\
g_{ur} &= 1,\\
g_{uy} &= -2\rho\bar{\rho}l\cos x(r^2 - 2mr - l^2 + a^2)\\
&\quad + 2\rho\bar{\rho}a\sin^2 x(mr + l^2),\\
g_{ry} &= -a\sin^2 x - 2l\cos x,\\
g_{xx} &= -r^2 - (l - a\cos x)^2,\\
g_{yy} &= \rho\bar{\rho}(r^2 - 2mr - l^2 + a^2)[a\sin^2 x + 2l\cos x]^2\\
&\quad - \rho\bar{\rho}\sin^2 x(r^2 + l^2 + a^2)^2.
\end{aligned} \tag{3.47}$$

Case II.B: $U^0 > 0$, $\beta^0 < -\frac{1}{4}(2)^{\frac{1}{2}}$. Now we use the rotation to set $U^0 = +\frac{1}{2}$ and get

$$\begin{aligned}
\beta^0 &= -\tfrac{1}{4}(2)^{\frac{1}{2}}\coth x,\\
\tau^0 &= -\tfrac{1}{2}ia(2)^{\frac{1}{2}}\sinh x,\\
\rho &= -(r - il + ia\cosh x)^{-1},\\
l^\mu &= (0, 1, 0, 0),\\
n^\mu &= \rho\bar{\rho}[r^2 + l^2 + a^2, \tfrac{1}{2}(r^2 + 2mr - l^2 + a^2), 0, a],\\
m^\mu &= -\tfrac{1}{2}(2)^{\frac{1}{2}}\bar{\rho}[-ia\sinh x + 2il\coth x, 0, 1, i\,\mathrm{csch}\,x],\\
g_{uu} &= -\rho\bar{\rho}(r^2 + 2mr - l^2 + a^2\cosh^2 x),\\
g_{ur} &= 1,\\
g_{uy} &= 2\rho\bar{\rho}l\cosh x(r^2 + 2mr - l^2 + a^2)\\
&\quad - 2\rho\bar{\rho}a\sinh^2 x(mr - l^2),\\
g_{ry} &= a\sinh^2 x - 2l\cosh x,\\
g_{xx} &= -r^2 - (-l + a\cosh x)^2,\\
g_{yy} &= -\rho\bar{\rho}(r^2 + 2mr - l^2 + a^2)(-a\sinh^2 x\\
&\quad + 2l\cosh x)^2 - \rho\bar{\rho}\sinh^2 x(r^2 + l^2 + a^2)^2.
\end{aligned} \tag{3.48}$$

[7] M. Demiański and E. Newman, Bull. Acad. Polon. Sci. **14**, 653 (1966).

Case II.C: $U^0 = +\frac{1}{2}$, $\beta^0 > -\frac{1}{4}(2)^{\frac{1}{2}}$:

$$\begin{aligned}
\beta^0 &= -\tfrac{1}{4}(2)^{\frac{1}{2}}\tanh x,\\
\tau^0 &= -\tfrac{1}{2}ia(2)^{\frac{1}{2}}\cosh x,\\
\rho &= -(r - il + ia\sinh x)^{-1},\\
l^\mu &= (0, 1, 0, 0),\\
n^\mu &= \rho\bar{\rho}[r^2 + l^2 - a^2, \tfrac{1}{2}(r^2 + 2mr - l^2 - a^2), 0, a],\\
m^\mu &= -\tfrac{1}{2}(2)^{\frac{1}{2}}\bar{\rho}(-ia\cosh x + 2il\tanh x, 0, 1, i\,\mathrm{sech}\,x),\\
g_{uu} &= -\rho\bar{\rho}(r^2 + 2mr - l^2 + a^2\sinh^2 x),\\
g_{ur} &= 1,\\
g_{uy} &= 2\rho\bar{\rho}l\sinh x(r^2 + 2mr - l^2 - a^2)\\
&\quad - 2\rho\bar{\rho}a\cosh^2 x(mr - l^2),\\
g_{ry} &= a\cosh^2 x - 2l\sinh x,\\
g_{xx} &= -r^2 - (-l + a\sinh x)^2,\\
g_{yy} &= -\rho\bar{\rho}(r^2 + 2mr - l^2 - a^2)(-a\cosh^2 x\\
&\quad + 2l\sinh x)^2 - \rho\bar{\rho}\cosh^2 x(r^2 + l^2 - a^2)^2.
\end{aligned} \tag{3.49}$$

Case II.D: $U^0 = +\frac{1}{2}$, $\beta^0 = -\frac{1}{4}(2)^{\frac{1}{2}}$:

$$\begin{aligned}
\beta^0 &= -\tfrac{1}{4}(2)^{\frac{1}{2}},\\
\tau^0 &= -\tfrac{1}{2}ia(2)^{\frac{1}{2}}e^x,\\
\rho &= -(r - il + iae^x)^{-1},\\
l^\mu &= (0, 1, 0, 0),\\
n^\mu &= \rho\bar{\rho}[r^2 + l^2, \tfrac{1}{2}(r^2 + 2mr - l^2), 0, a],\\
m^\mu &= -\tfrac{1}{2}(2)^{\frac{1}{2}}\bar{\rho}(-iae^x + 2il, 0, 1, ie^{-x}),\\
g_{uu} &= -\rho\bar{\rho}(r^2 + 2mr - l^2 + a^2e^{2x}),\\
g_{ur} &= 1,\\
g_{uy} &= 2\rho\bar{\rho}le^x(r^2 + 2mr - l^2) - 2\rho\bar{\rho}ae^{2x}(mr - l^2),\\
g_{ry} &= ae^{2x} - 2le^x,\\
g_{xx} &= -r^2 - (-l + ae^x)^2,\\
g_{yy} &= -\rho\bar{\rho}(r^2 + 2mr - l^2)(-ae^{2x} + 2le^x)^2\\
&\quad - \rho\bar{\rho}(r^2 + l^2)^2e^{2x},
\end{aligned} \tag{3.50}$$

Case II.E: $U^0 = 0$, $l \neq 0$. We may use a tetrad rotation and a rescaling of coordinates to set $l = +1$. Then the solution is

$$\begin{aligned}
\beta^0 &= -\tfrac{1}{4}(2)^{\frac{1}{2}}x^{-1},\\
\tau^0 &= -\tfrac{1}{2}i(2)^{\frac{1}{2}}x,\\
\rho &= -(r + ib + \tfrac{1}{2}ix^2)^{-1},\\
l^\mu &= (0, 1, 0, 0),\\
n^\mu &= \rho\bar{\rho}(r^2 + b^2, mr + b, 0, 1),\\
m^\mu &= -\tfrac{1}{2}(2)^{\frac{1}{2}}\bar{\rho}(-\tfrac{1}{4}ix^3 - ibx, 0, 1, ix^{-1}),\\
g_{uu} &= -\rho\bar{\rho}(2mr + 2b + x^2),\\
g_{ur} &= 1,\\
g_{uy} &= \rho\bar{\rho}x^2(r^2 - 2mbr - \tfrac{1}{2}mrx^2 - b^2 - \tfrac{1}{2}bx^2),\\
g_{ry} &= bx^2 + \tfrac{1}{4}x^4,\\
g_{xx} &= -r^2 - (b + \tfrac{1}{2}x^2)^2,\\
g_{yy} &= -\rho\bar{\rho}(2mr + 2b)(bx^2 + \tfrac{1}{4}x^4)^2 - \rho\bar{\rho}x^2(r^2 + b^2)^2.
\end{aligned} \tag{3.51}$$

Case II.F: $U^0 = 0$, $l = 0$:

$$\begin{aligned}
\beta^0 &= 0,\\
\tau^0 &= -\tfrac{1}{2}i(2)^{\frac{1}{2}},\\
\rho &= -(r + ix)^{-1},\\
l^\mu &= (0, 1, 0, 0),\\
n^\mu &= \rho\bar{\rho}(r^2, mr - \tfrac{1}{2}, 0, 1),\\
m^\mu &= -\tfrac{1}{2}(2)^{\frac{1}{2}}\bar{\rho}(-ix^2, 0, 1, i),\\
g_{uu} &= -2\rho\bar{\rho}mr,\\
g_{ur} &= 1,\\
g_{uy} &= \rho\bar{\rho}(r^2 - 2mrx^2 + x^2),\\
g_{ry} &= x^2,\\
g_{xx} &= -r^2 - x^2,\\
g_{yy} &= -\rho\bar{\rho}(r^4 + 2mx^4r - x^4).
\end{aligned} \tag{3.52}$$

Case III: $\pi^0 \neq 0$. Now we choose θ^0 such that π^0 is everywhere real. Equations (3.16), (3.17), (3.30), and (3.42) imply that

$$\begin{aligned}
\mu^0 &= -2\pi^0(\beta^0 + \bar{\beta}^0),\\
\beta^0 - \bar{\beta}^0 &= 2i\rho^0\pi^0,\\
\gamma^0 - \bar{\gamma}^0 &= -2i\rho^0(\pi^0)^2,\\
\alpha^0 &= -\beta^0.
\end{aligned}$$

Likewise, Eqs. (3.26), (3.27), and (3.37) reduce to

$$\begin{aligned}
M^0 - \bar{M}^0 &= 4i\rho^0\pi^0(\beta^0 + \bar{\beta}^0) - 2\pi^0(\tau^0 - \bar{\tau}^0),\\
\tau^0 + \bar{\tau}^0 &= 4(\rho^0)^2\pi^0,\\
\psi^0 - \bar{\psi}^0 &= 2i\rho^0(M^0 + \bar{M}^0)\\
&\quad + 2(\tau^0 - \bar{\tau}^0)(\beta^0 + \bar{\beta}^0)\\
&\quad - 6i(\rho^0)^3(\pi^0)^2.
\end{aligned}$$

It is advantageous to abandon the complex notation at this stage and work with real and imaginary parts. Let

$$\begin{aligned}
\beta^0 &= b^0 + i\rho^0\pi^0,\\
\tau^0 &= 2(\rho^0)^2\pi^0 + i\pi^0t^0,\\
\mu^0 &= -4\pi^0b^0,\\
\gamma^0 &= 2\pi^0b^0 - i\rho^0(\pi^0)^2,\\
M^0 &= -U^0 + 4(\rho^0)^2(\pi^0)^2 - 2i(\pi^0)^2t^0 - 4i\rho^0\pi^0b^0,\\
\psi^0 &\equiv m^0 + il^0\\
&= m^0 + i[-2\rho^0U^0 + 4b^0\pi^0t^0 + 2(\rho^0)^3(\pi^0)^2].
\end{aligned} \tag{3.53}$$

Then the equations to solve are

$$\xi^{0i}\rho^0_{,i} = \bar{\xi}^{0i}\rho^0_{,i} = \pi^0t^0, \tag{3.54}$$

$$\xi^{0i}t^0_{,i} = \bar{\xi}^{0i}t^0_{,i} = -8(\rho^0)^3\pi^0, \tag{3.55}$$

$$\xi^{0i}\pi^0_{,i} = \bar{\xi}^{0i}\pi^0_{,i} = 2b^0\pi^0, \tag{3.56}$$

$$\xi^{0i}b^0_{,i} = \bar{\xi}^{0i}b^0_{,i} = \tfrac{1}{2}U^0 - 2(b^0)^2 - \tfrac{9}{2}(\rho^0)^2(\pi^0)^2, \tag{3.57}$$

$$\begin{aligned}
\xi^{0i}U^0_{,i} &= \bar{\xi}^{0i}U^0_{,i}\\
&= -3m^0\pi^0 - 6\rho^0(\pi^0)^3t^0 - 12(\rho^0)^2(\pi^0)^2b^0,
\end{aligned} \tag{3.58}$$

$$\xi^{0i}\psi^0_{,i} = \bar{\xi}^{0i}\psi^0_{,i} = 6i\rho^0\pi^0\psi^0, \tag{3.59}$$

$$\bar{\xi}^{0i}\xi^{0j}_{,i} - \xi^{0i}\bar{\xi}^{0j}_{,i} = -2i\rho^0X^{0j} - 2b^0(\xi^{0j} - \bar{\xi}^{0j}), \tag{3.60}$$

$$\xi^{0i}X^{0j}_{,i} - X^{0i}\xi^{0j}_{,i} = -2i\rho^0(\pi^0)^2(\xi^{0j} - \bar{\xi}^{0j}), \tag{3.61}$$

$$\begin{aligned}
X^{0i}\rho^0_{,i} &= X^{0i}t^0_{,i} = X^{0i}\pi^0_{,i}\\
&= X^{0i}b^0_{,i} = X^{0i}U^0_{,i} = X^{0i}\psi^0_{,i} = 0.
\end{aligned}$$

Again by Eq. (3.44) we can make ξ^{01}, ξ^{04} imaginary and $\xi^{03} = d\pi^0$, where d is a real constant to be chosen in a moment. Let $x^3 = x$. Equations (3.54) and (3.55) imply

$$\rho^0_{,xx} = -8(\rho^0)^3/d^2. \tag{3.62}$$

The solution is $\rho^0 = a\,\mathrm{cn}\,\{[2a(2)^{\frac{1}{2}}/d]x\}$ where cn is an elliptic function of modulus $k = \frac{1}{2}(2)^{\frac{1}{2}}$ and a is the constant of integration.

Case III.A: $a = 0$. Here we choose $d = +1$. The remaining integrations are trivial and lead to the following vacuum solution:

$$\begin{aligned}
\tau^0 &= 0,\\
m^0 &= m,\\
l^0 &= 0,\\
\pi^0 &= \tfrac{1}{2}(2)^{\frac{1}{2}}f(x),\\
l^\mu &= (0, 1, 0, 0),\\
n^\mu &= \{1, \tfrac{1}{2}r^2[f(x - 1/r)]^2, 0, 0\},\\
m^\mu &= \{0, \tfrac{1}{2}(2)^{\frac{1}{2}}rf(x), -\tfrac{1}{2}(2)^{\frac{1}{2}}r^{-1}f(x),\\
&\quad -\tfrac{1}{2}i(2)^{\frac{1}{2}}r^{-1}[f(x)]^{-1}\},
\end{aligned} \tag{3.63}$$

$$\begin{aligned}
g_{uu} &= -r^2[f(x - 1/r)]^2,\\
g_{ur} &= 1,\\
g_{ux} &= -r^2,\\
g_{xx} &= -r^2[f(x)]^{-2},\\
g_{yy} &= -r^2[f(x)]^2,
\end{aligned} \tag{3.64}$$

where

$$f(x) = (-2mx^3 + ax + b)^{\frac{1}{2}}$$

and m, a, b are constants.

This solution is the static "C" metric discussed by Ehlers and Kundt.[8]

Case III.B: $a \neq 0$. Choose $d = -2a(2)^{\frac{1}{2}}$. Then

$$\begin{aligned}
\rho^0 &= a\,\mathrm{cn}\,x,\\
t^0 &= 2a^2(2)^{\frac{1}{2}}\,\mathrm{sn}\,x\,\mathrm{dn}\,x.
\end{aligned} \tag{3.65}$$

Equation (3.59) is next integrated to yield

$$\psi^0 = (m + il)(\mathrm{dn}\,x - \tfrac{1}{2}i(2)^{\frac{1}{2}}\,\mathrm{sn}\,x)^3, \tag{3.66}$$

[8] J. Ehlers and W. Kundt in *Gravitation: An Introduction to Current Research*, L. Witten, Ed. (John Wiley & Sons, Inc., New York, 1962).

where m and l are constants. Equation (3.58) can be rewritten as

$$\xi^{0i}[U^0 + 3(\rho^0\pi^0)^2]_{,i} = -3m^0\pi^0,$$

and integrated to yield

$$U^0 + 3(\rho^0\pi^0)^2 = b + \tfrac{3}{4}(2)^{\frac{1}{2}}a^{-1}\,\mathrm{cn}\,x(m\,\mathrm{sn}\,x - l(2)^{\frac{1}{2}}\,\mathrm{dn}\,x), \quad (3.67)$$

introducing a constant b. When Eqs. (3.56), (3.57), and (3.67) are combined, they give the following equation for $(\pi^0)^2$:

$$(\pi^0)^2_{,x}\,\mathrm{sn}\,x\,\mathrm{dn}\,x - (\pi^0)^2\,\mathrm{cn}^3\,x = -\tfrac{1}{4}ba^{-2}\,\mathrm{cn}\,x + \tfrac{1}{4}la^{-3}\,\mathrm{dn}^3\,x + \tfrac{1}{16}(2)^{\frac{1}{2}}ma^{-3}\,\mathrm{sn}^3\,x, \quad (3.68)$$

which has the solution

$$(\pi^0)^2 = c\,\mathrm{sn}\,x\,\mathrm{dn}\,x + \tfrac{1}{4}ba^{-2}\,\mathrm{cn}^2\,x - \tfrac{1}{8}(2)^{\frac{1}{2}}a^{-3}\,\mathrm{cn}\,x(m\,\mathrm{sn}\,x + l(2)^{\frac{1}{2}}\,\mathrm{dn}\,x). \quad (3.69)$$

Finally, the solution of Eqs. (3.60), (3.61), for $j = 1, 4$, is

$$X^{0j} = D^j\,\mathrm{sn}\,x + E^j\,\mathrm{dn}\,x, \quad (3.70)$$

$$\xi^{0j} = \tfrac{1}{2}i(2)^{\frac{1}{2}}(\pi^0)^{-1}(-D^j\,\mathrm{dn}\,x + \tfrac{1}{2}E^j\,\mathrm{sn}\,x). \quad (3.71)$$

We choose $D^j = \delta_{j4}$ and $E^j = \delta_{j1}$, and the resulting vacuum solution is

$$\rho = -(r + ia\,\mathrm{cn}\,x)^{-1},$$
$$l^\mu = (0, 1, 0, 0),$$
$$n^\mu = (X^1, U, 0, X^4),$$
$$m^\mu = -\tfrac{1}{2}(2)^{\frac{1}{2}}\bar{\rho}[-\tfrac{1}{2}i(\pi^0)^{-1}\,\mathrm{sn}\,x, (2)^{\frac{1}{2}}\pi^0 \times (r^2 + 3a^2\,\mathrm{cn}^2\,x), 4a\pi^0, i(\pi^0)^{-1}\,\mathrm{dn}\,x],$$

where

$$X^1 = \mathrm{dn}\,x + (2)^{\frac{1}{2}}a\rho\bar{\rho}(r\,\mathrm{cn}\,x + a(2)^{\frac{1}{2}}\,\mathrm{sn}\,x\,\mathrm{dn}\,x)\,\mathrm{sn}\,x,$$
$$X^4 = \mathrm{sn}\,x - 2(2)^{\frac{1}{2}}a\rho\bar{\rho}(r\,\mathrm{cn}\,x + a(2)^{\frac{1}{2}}\,\mathrm{sn}\,x\,\mathrm{dn}\,x)\mathrm{dn}\,x,$$
$$U = b + \tfrac{3}{4}(2)^{\frac{1}{2}}a^{-1}\,\mathrm{cn}\,x(m\,\mathrm{sn}\,x - l(2)^{\frac{1}{2}}\,\mathrm{dn}\,x) + 2(2)^{\frac{1}{2}}acr\,\mathrm{cn}^3\,x - a^{-1}br(2)^{\frac{1}{2}}\,\mathrm{sn}\,x\,\mathrm{cn}\,x\,\mathrm{dn}\,x - \tfrac{1}{2}a^{-2}mr(\mathrm{dn}^3\,x - \tfrac{3}{2}\,\mathrm{sn}^2\,x\,\mathrm{dn}\,x) + \tfrac{1}{2}a^{-2}lr(\tfrac{3}{2}\,\mathrm{dn}^2\,x\,\mathrm{sn}\,x - \tfrac{1}{4}\mathrm{sn}^3\,x) + (\pi^0)^2(r^2 - 3a^2\,\mathrm{cn}^2\,x) + \rho\bar{\rho}(rm^0 + al^0\,\mathrm{cn}\,x) - 4\rho\bar{\rho}a^2(\pi^0)^2(r\,\mathrm{cn}\,x - a(2)^{\frac{1}{2}}\,\mathrm{sn}\,x\,\mathrm{dn}\,x)^2, \quad (3.72)$$
$$m^0 = m(\mathrm{dn}^3\,x - \tfrac{3}{2}\mathrm{dn}\,x\,\mathrm{sn}^2\,x) + l(2)^{\frac{1}{2}}(\tfrac{3}{2}\mathrm{dn}^2\,x\,\mathrm{sn}\,x - \tfrac{1}{4}\mathrm{sn}^3 x),$$
$$l^0 = -m(2)^{\frac{1}{2}}(\tfrac{3}{2}\mathrm{dn}^2\,x\,\mathrm{sn}\,x - \tfrac{1}{4}\mathrm{sn}^3\,x) + l(\mathrm{dn}^3\,x - \tfrac{3}{2}\mathrm{dn}\,x\,\mathrm{sn}^2\,x),$$
$$(\pi^0)^2 = c\,\mathrm{sn}\,x\,\mathrm{dn}\,x + \tfrac{1}{4}a^{-2}b\,\mathrm{cn}^2\,x - \tfrac{1}{8}(2)^{\frac{1}{2}}a^{-3}\,\mathrm{cn}\,x(m\,\mathrm{sn}\,x + l(2)^{\frac{1}{2}}\,\mathrm{dn}\,x),$$

and a, b, c, l, m are all arbitrary constants.

The nonzero metric components in these terms are

$$g_{uu} = -2U\,\mathrm{dn}^2\,x - (X^4\pi^0)^2(r^2 + a^2\,\mathrm{cn}^2\,x)$$
$$g_{ur} = \mathrm{dn}\,x$$
$$g_{ux} = -\tfrac{1}{4}(2)^{\frac{1}{2}}a^{-1}\,\mathrm{dn}\,x(r^2 + 3a^2\,\mathrm{cn}^2\,x)$$
$$g_{uy} = -U\,\mathrm{sn}\,x\,\mathrm{dn}\,x + X^1X^4(\pi^0)^2(r^2 + a^2\,\mathrm{cn}^2\,x)$$
$$g_{ry} = \tfrac{1}{2}\mathrm{sn}\,x \quad (3.73)$$
$$g_{xx} = -\tfrac{1}{16}(a\pi^0)^{-2}(r^2 + a^2\,\mathrm{cn}^2\,x)$$
$$g_{xy} = -\tfrac{1}{8}(2)^{\frac{1}{2}}a^{-1}\,\mathrm{sn}\,x(r^2 + 3a^2\,\mathrm{cn}^2\,x)$$
$$g_{yy} = -\tfrac{1}{2}U\,\mathrm{sn}^2\,x - (X^1\pi^0)^2(r^2 + a^2\,\mathrm{cn}^2\,x).$$

4. SOLUTION FOR $\rho = 0$

In what follows we can assume $\mu = 0$ as well, because otherwise after interchange of l^μ and n^μ the previous derivation would apply. Since l^μ is now proportional to a gradient, we can follow Newman and Penrose[4] and set $\tau = \bar{\alpha} + \beta$, $X^1 = 1$, $\xi^1 = 0$. Furthermore, Eqs. (2.4d), (2.9), (2.10) imply $D\tau = 0$, $D\pi = 0$, and $\pi\bar{\pi} = \tau\bar{\tau}$, so we may use the tetrad rotation Eq. (3.38) to set $\tau = -\pi$. The NP equations (2.4f), (2.5b), (2.5d), (2.6a) now yield an expression for ψ, namely,

$$\psi = 2\tau(\beta - \alpha). \quad (4.1)$$

We must insist on $\psi \neq 0$ and hence $\tau \neq 0$. Some of the other immediate consequences of the equations are

$$D\psi = \Delta\psi = 0, \quad (4.2)$$

$$D\tau = \Delta\tau = 0, \quad (4.3)$$

$$\delta\psi = \bar{\delta}\psi = 3\tau\psi, \quad (4.4)$$

$$\delta\tau = \bar{\delta}\tau = 2\beta\tau, \quad (4.5)$$

$$\alpha + \beta = \bar{\alpha} + \bar{\beta}, \quad (4.6)$$

$$\gamma = \bar{\gamma}, \quad (4.7)$$

$$\delta\gamma = 0. \quad (4.8)$$

The radial integration is easily performed. All the variables are independent of r except

$$\gamma = \gamma^0 + r[(\tau + \bar{\tau})(\beta - \alpha) - \tau^2], \quad (4.9)$$

$$X^i = X^{0i} - (r - \bar{\tau})(\xi^i - \bar{\xi}^i), \quad (4.10)$$

$$\omega = \omega^0 - r(\tau + \bar{\tau}), \quad (4.11)$$

$$U = U^0 - r[2\gamma^0 + (\tau - \bar{\tau})\omega^0] - r^2[(\tau + \bar{\tau})(\beta - \alpha) - \tau^2]. \quad (4.12)$$

When these are substituted in the remaining NP

equations we get the following:

$$\delta\gamma^0 = -\omega^0[(\tau + \bar{\tau})(\beta - \alpha) - \tau^2], \quad (4.13)$$

$$\delta U^0 - X^{0j}\omega^0_{,j} = \omega^0[2\gamma^0 + (\tau - \bar{\tau})(\omega^0 - \bar{\omega}^0)] - U^0(\tau + \bar{\tau}), \quad (4.14)$$

$$\delta\omega^0 - \delta\bar{\omega}^0 = -(\omega^0 - \bar{\omega}^0)(\alpha + 2\beta + \bar{\beta}), \quad (4.15)$$

$$\bar{\delta}\xi^i - \delta\bar{\xi}^i = (\xi^i - \bar{\xi}^i)(\alpha - \bar{\beta}), \quad (4.16)$$

$$\delta X^{0i} - X^{0j}\xi^i_{,j} = \omega^0(\tau - \bar{\tau})(\xi^i - \bar{\xi}^i). \quad (4.17)$$

First we will show how ω^0 may be eliminated. The coordinate transformation $r \to r + f(x^1, x^3, x^4)$ leaves previous conditions unchanged. Under this transformation

$$\gamma^0 \to \gamma^0 - f[(\tau + \bar{\tau})(\beta - \alpha) - \tau^2], \quad (4.18)$$

$$\omega^0 \to \omega^0 + \delta f + f(\tau + \bar{\tau}). \quad (4.19)$$

The quantity in brackets is $D\gamma$. If $D\gamma$ is nonzero, $f = \gamma^0/D\gamma$ will make $\gamma^0 \to 0$ and Eq. (4.13) will then imply $\omega^0 \to 0$. If $D\gamma = 0$ we have $\delta\gamma^0 = 0$. Then Eq. (4.19) may be used to make $\omega^0 \to 0$, provided the integrability conditions are satisfied. In other words we must specify Df, Δf such that all the commutators applied to f are given correctly. Choose $Df = 0$, $X^{0j}f_{,j} = U^0 - 2\gamma^0 f$. The only nontrivial commutators are $(\Delta\delta - \delta\Delta)f$ and $(\bar{\delta}\delta - \delta\bar{\delta})f$; and these are automatically satisfied by virtue of Eqs. (4.14)–(4.17).

Next we show how to eliminate U^0, γ^0 by means of a combined coordinate transformation and tetrad rotation. The rotation is

$$(l')^\mu = A^{-1}(x^1)l^\mu,$$
$$(n')^\mu = A(x^1)n^\mu,$$

and the change of coordinates is

$$x^{1'} = \int_0^{x^1} A^{-1}(u)\,du,$$
$$r' = rA(x^1) + U^0R(x^1),$$

which together preserve all previous conditions but send $U = U^0 - 2r\gamma^0(x^1) - r^2D\gamma$ into something new. We want to pick A, R such that the new U^0, γ^0 are zero. The observation that $\delta(U^0D\gamma) = 0$ is sufficient to reduce the problem to the solution of two total differential equations for $A(x^1)$, $R(x^1)$, given γ^0 and $U^0D\gamma$ as arbitrary functions of x^1. Under sufficient assumptions of continuity, such equations always have solutions, which is all we need to know.

Finally, from $\delta\psi = \bar{\delta}\psi \neq 0$ we can choose a coordinate $x^3 = x$ such that ξ^3 is real, and then the usual transformation $x^4 \to x^4 + f(x^3, x^4)$ makes ξ^4 imaginary. Equations (4.2) and (4.3) show that the remaining variables depend only on x.

From Eqs. (4.5) and (4.6), we find

$$\begin{aligned}\tau - \bar{\tau} &= \alpha - \bar{\alpha} + \beta + \bar{\beta} \\ &= 2(\beta - \bar{\beta}) \\ &= \tau^{-1}\,\delta\tau - \bar{\tau}^{-1}\delta\bar{\tau}.\end{aligned} \quad (4.20)$$

Solve Eq. (4.4) for τ and substitute in this expression. The result may be written as

$$0 = \delta\left(\frac{\psi^{\frac{4}{3}}\delta\bar{\psi}}{\bar{\psi}^{\frac{4}{3}}\delta\psi}\right) \quad (4.21)$$

and integrated twice to give

$$C\bar{\psi}^{-\frac{1}{3}} = \psi^{-\frac{1}{3}} + D. \quad (4.22)$$

The coordinate freedom $x' = f(x)$ would let us set Re (ψ) equal to any specified function of x, but thanks to Eq. (4.22) we can choose x such that

$$\psi = (m + il)(x + ia)^{-3}, \quad (4.23)$$

where m, l, a are again real constants. Next, τ, α, and β are all expressed in terms of ξ^3 and substituted into Eq. (4.1) which becomes

$$[(\xi^3)^2]_{,x} + \frac{2ia(\xi^3)^2}{x^2 + a^2} = -\frac{m + il}{(x + ia)^2}. \quad (4.24)$$

If $a \neq 0$, this has the real solution

$$(\xi^3)^2 = \frac{2amx + l(a^2 - x^2)}{2a(x^2 + a^2)}, \quad (4.25)$$

while if $a = 0$ the solution is

$$(\xi^3)^2 = C + m/x, \quad (4.26)$$

where C is an arbitrary constant, and necessarily $l = 0$. Then by a coordinate transformation we can set $C = \pm\frac{1}{2}, 0$. The resulting metrics are

Case IV.A:

$$l^\mu = (0, 1, 0, 0),$$
$$n^\mu = \left(1, \frac{-r^2 l}{2a(x^2 + a^2)}, 0, \frac{4ar}{x^2 + a^2}\right), \quad (4.27)$$
$$m^\mu = \left(0, \frac{2rx\xi}{x^2 + a^2}, \xi, \frac{i}{\xi}\right),$$

$$\begin{aligned} g_{uu} &= r^2 l a^{-1}(x^2 + a^2)^{-1}, \\ g_{ur} &= 1, \\ g_{ux} &= -2rx(x^2 + a^2)^{-1}, \\ g_{xx} &= -\tfrac{1}{2}\xi^{-2}, \\ g_{vv} &= -2\xi^2, \end{aligned} \quad (4.28)$$

where

$$\xi = \left[\frac{2amx + l(a^2 - x^2)}{2a(x^2 + a^2)}\right]^{\frac{1}{2}}. \quad (4.29)$$

Case IV.B:

$$\begin{aligned} l^\mu &= (0, 1, 0, 0), \\ n^\mu &= (1, Cr^2/x^2, 0, 0), \\ m^\mu &= (0, 2r\xi/x, \xi, i/\xi), \\ g_{uu} &= -2Cr^2/x^2, \\ g_{ur} &= 1, \\ g_{ux} &= -2r/x, \\ g_{xx} &= -\tfrac{1}{2}\xi^{-2}, \\ g_{vv} &= -2\xi^2, \end{aligned} \tag{4.30}$$

where

$$\begin{aligned} C &= \pm\tfrac{1}{2}, 0, \\ \xi &= (C + m/x)^{\frac{1}{2}}. \end{aligned} \tag{4.31}$$

5. DISCUSSION

The solutions of Case II, Eqs. (3.46)–(3.53), are the easiest ones to try to interpret physically. If we examine the two-dimensional positive-definite metric of the wavefronts or equipotentials $u = \text{const}$, $r = \text{const}$, we see that asymptotically as $r \to \infty$ they become spheres in Case II.A, pseudospheres in Cases II.B–II.D, and planes in Cases II.E, II.F. Case II.A is Kerr–NUT space, which Demiański and Newman[7] maintain is the field of a particle possessing mass, angular momentum, and a "magnetic monopole of mass." We propose that all the metrics of Case II represent spinning particles and correspond to the six different ways we can pick a velocity four-vector and an angular-momentum vector orthogonal to it. We attribute Cases II.B, II.D to a particle with spacelike velocity and Cases II.E, II.F to one with lightlike velocity. The angular-momentum vector is supposed to be spacelike for Cases II.A, II.C, II.F null for Cases II.D, II.E, and timelike for Case II.B. These assertions are reinforced by an examination of the geometry of the principal congruences in the flat-space limit $m = l = 0$, and also from the fact that the metrics may be obtained from one another by infinite Lorentz transformations. Particles with the above properties have been discussed in the framework of quantum mechanics by Wigner.[9]

Case II.A, Eqs. (3.63) and (3.64), is the static degenerate "C" metric listed by Ehlers and Kundt.[8] No suitable interpretation is known. Case II.B seems to be closely related, but with rotation added. Both are asymptotically flat at $r \to \infty$. Case II.B is believed to be new.

Case IV.B, Eqs. (4.29) and (4.30), also appears in Ehlers and Kundt,[8] referred to there as the "B" metrics. Case IV.A is a rotating generalization which tends smoothly to IV.B in the limit $l \to 0$, $a \to 0$, $l/a \to C$.

In a search for a subclass of metrics with two Killing vectors, Carter[10] has found type D metrics equivalent to II and IV although he did not attempt to delineate the many cases.

6. ACKNOWLEDGMENTS

I would like to thank Dr. Jon Mathews and Dr. Kip S. Thorne for help and encouragement in this work.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

$SU(6)$ Clebsch–Gordan Coefficients for the Product $35 \otimes 70$

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(Received 4 August 1968)

A method is presented which makes explicit use of Young diagrams to calculate $SU(3) \otimes SU(2)$ multiplet-coupling coefficients in $SU(6)$. The multiplet-coupling coefficients for $\mathbf{35} \otimes \mathbf{70}$ are given.

INTRODUCTION

In this paper we present the method used previously to calculate the $SU(6)$ multiplet-coupling coefficients for the product $\mathbf{35} \otimes \mathbf{56}$.[1] As an example of the use of the method, we give here the previously unpublished coefficients for $\mathbf{35} \otimes \mathbf{70}$. These coefficients have been used to calculate decay widths[2] and to construct the irreducible mass tensors of the **20** representation in bootstrap calculations.[3] They can be used to calculate scattering amplitudes for such processes as a meson + baryon → meson + baryon resonance, where the baryon resonance is accommodated in the **70** representation of $SU(6)$.

The group $SU(6)$, which is used to classify the elementary particles, contains $SU(3)$, whose states give the isotopic spin and hypercharge quantum numbers of the particles, and $SU(2)$, whose states give the intrinsic spin. Multiplet-coupling coefficients have been published for the $SU(3)$ products $8 \otimes 8$ and $8 \otimes 10$, which are the $SU(3)$ multiplets in which the most interesting particles and resonances have been accommodated.[4] Our procedure makes use of these existing tables, the Condon–Shortley tables for $SU(2)$, and the permutation symmetries of states in $SU(6)$ to compute the multiplet-coupling coefficients for the $\mathbf{35} \otimes \mathbf{70}$ of $SU(6)$. We have used the tables for $SU(3)$ and $SU(2)$ to write out highest-weight $SU(3) \otimes SU(2)$ states of $SU(6)$. These states do not, in general, belong to irreducible representations of $SU(6)$. We have then derived information about the permutation symmetry of the irreducible representations of $SU(6)$ from their Young tableaux. [It is well known that operators of the permutation groups commute with operators of the unitary groups, so that the states of $SU(6)$ can be classified according to their mixed symmetries under quark intercharge. The mixed symmetries are characterized by the use of Young tableaux.] This procedure has yielded the equations necessary to calculate the multiplet-coupling coefficients (or generalized Clebsch–Gordan coefficients) for the irreducible representations of $\mathbf{35} \otimes \mathbf{56}$ and $\mathbf{35} \otimes \mathbf{70}$.

THE FORMATION OF PRODUCT STATES IN QUARK FORM

To calculate the coefficients it is necessary to know what irreducible representations occur in the $SU(6)$ product space. Here $\mathbf{35} \otimes \mathbf{70} = \mathbf{20} \oplus \mathbf{56} \oplus \mathbf{70} \oplus \mathbf{540} \oplus \mathbf{560} \oplus \mathbf{1134}$.[5] One next determines the $SU(3) \otimes SU(2)$ composition of the product representations. An $SU(3) \otimes SU(2)$ representation is specified by the notation $N^m = \{SU(3)^{SU(2)}\}$. The representations whose direct product is being taken will hereinafter be referred to as parent representations. The $SU(6)$ **35** contains the N^m multiplets 8^3, 8^1, and 1^3. The **70** contains 8^4, 10^2, 8^2, and 1^2. The $SU(3) \otimes SU(2)$ representations [unreduced in $SU(6)$] which occur in the product are formed by taking all possible products of the parents. Thus, for $\mathbf{35} \otimes \mathbf{70}$ we form all product spaces [reduced in $SU(3)$ and $SU(2)$] allowed by the following scheme:

$$\mathbf{35} \otimes \mathbf{70} = \begin{Bmatrix} 8^3 \\ 8^1 \\ 1^3 \end{Bmatrix} \otimes \begin{Bmatrix} 10^2 \\ 8^4 \\ 8^2 \\ 1^2 \end{Bmatrix}. \tag{1}$$

For example,

$$(8^3 \otimes 10^2) = 8^{2,4} \oplus 10^{2,4} \oplus 27^{2,4} \oplus 35^{2,4}.$$

In general, an $SU(3) \otimes SU(2)$ representation which is also reduced in $SU(6)$ contains a mixture of products coming from (1). For example, the N^m state 35^2 is given by

$$35^2 = (8^3 \otimes 10^2) \oplus (8^1 \otimes 10^2). \tag{2}$$

* Supported in part by the National Science Foundation.

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The quantum numbers which classify states in $SU(6) \supset SU(3) \otimes SU(2)$ are S (ordinary spin), S_z, I (I-spin), I_z, and Y (hypercharge). A highest-weight state is here taken to be the state of a representation which has highest S_z, then I_z, then Y. We can form the state of highest weight in the $SU(3)^{SU(2)}$ $35^2 = (8^3 \otimes 10^2)$ by using the $SU(3)$ coupling coefficients of Chilton–McNamee,[5] and the $SU(2)$ coefficients of Condon–Shortley. Thus, the highest-weight state in $8 \otimes 10$ of multiplicity N in $SU(3)$ is

$$\phi_{35}(1\ \tfrac{5}{2};\ \tfrac{5}{2}) = \phi_8(0\ 1;\ 1)\phi_{10}(1\ \tfrac{3}{2};\ \tfrac{3}{2}), \qquad (3)$$

where $\phi_N(Y, I; I_z)$ is a state belonging to the N-dimensional representation of $SU(3)$. For $3 \otimes 2$ in $SU(2)$,

$$\Psi_2(\tfrac{1}{2};\ \tfrac{1}{2}) = (\tfrac{1}{3})^{\frac{1}{2}}[(2)^{\frac{1}{2}}\Psi_3(1;\ 1)\Psi_2(\tfrac{1}{2};\ -\tfrac{1}{2}) - \Psi_3(1;\ 0)\Psi_2(\tfrac{1}{2};\ \tfrac{1}{2})], \qquad (4)$$

where $\Psi_m(S; S_z)$ is a state of the m dimensional representation of $SU(2)$. Hence, in $SU(6)$ for $8^3 \otimes 8^2 = 35^2$, the highest-weight state is

$$\Phi(1\ \tfrac{5}{2}\ \tfrac{1}{2};\ \tfrac{5}{2}\ \tfrac{1}{2}) = (\tfrac{1}{3})^{\frac{1}{2}}[(2)^{\frac{1}{2}}\Phi(0\ 1\ 1;\ 1\ 1)\Phi(1\ \tfrac{3}{2}\ \tfrac{1}{2};\ \tfrac{3}{2}\ -\tfrac{1}{2}) - \Phi(0\ 1\ 1;\ 1\ 0)\Phi(1\ \tfrac{3}{2}\ \tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2}), \qquad (5)$$

where

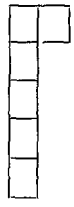
$$\Phi(Y, I, S; I_z, S_z) = \phi(Y, I, I_z)\Psi(S, S_z).$$

The 35^2 which arises from $(8^1 \otimes 10^2)$ can be formed in a similar fashion. The most general form of the state of highest weight of the 35^2 in **35** $\otimes$ **70** is, therefore,

$$\Phi(1\ \tfrac{5}{2}\ \tfrac{1}{2};\ \tfrac{5}{2}\ \tfrac{1}{2}) = \alpha\Phi_1(1\ \tfrac{5}{2}\ \tfrac{1}{2};\ \tfrac{5}{2}\ \tfrac{1}{2}) + \beta\Phi_2(1\ \tfrac{5}{2}\ \tfrac{1}{2};\ \tfrac{5}{2}\ \tfrac{1}{2}), \qquad (6)$$

where Φ_1 comes from $(8^3 \otimes 10^2)$ and Φ_2 from $(8^1 \otimes 10^2)$. Since the 35^2 contains a mixture of the **560** and **1134** representations of $SU(6)$, a proper choice of the multiplet-coupling factors α and β will serve to reduce the 35^2 into one or the other $SU(6)$ representation. α and β, when thus determined, are the generalized Clebsch–Gordan coefficients (or multiplet-coupling factors) for reducing 35^2 into the $SU(6)$ representations **560** and **1134**. The values of α and β which reduce 35^2 will be calculated in this paper as an example of the method herein presented. The proper choice of coefficients was made by writing the state of highest weight in explicit quark form and imposing the permutation symmetry of the $SU(6)$ product representation on the quarks.

For this it is necessary to have the parent representations in quark form. The fundamental 6-dimensional (quark) representation of $SU(6)$ will be written in the form $(p_+, n_+, \lambda_+, p_-, n_-, \lambda_-)$. The conjugate representation is chosen to be $(\bar{p}_-, -\bar{n}_-, -\bar{\lambda}_-, -\bar{p}_+, \bar{n}_+, \bar{\lambda}_+)$. (Note that $\bar{p}_+$ is an antiproton with spin *up*.) The Young diagram of the **35** is

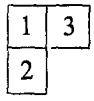


and of the **70** is

In tensor notation, the **35** is thus the traceless tensor $T^{\alpha}_{\beta} - \frac{1}{6}T^{\mu}_{\mu}$ and the **70** is

$$T_{[\alpha\beta]\gamma} + T_{[\gamma\beta]\alpha}.$$

The state of highest weight of the **35** is therefore $p_+\bar{n}_+$, which belongs to 8^3. The state of highest weight of the **70** is $(\frac{1}{2})^{\frac{1}{2}}[p_+\lambda_+]p_+$, which belongs to 8^4, where we use the standard tableaux



and the definition of a Young operator given in Hamermesh,[6] $Y = QP = \sum_{qp}(-1)^q qp$. All the states of a given $SU(3) \otimes SU(2)$ representation can be generated from the state of highest weight by making use of the generators[7]

$$I_{\pm} = \sum_q I_q^{\pm} + \sum_{\bar{q}} I_{\bar{q}}^{\pm}, \quad V_{\pm} = \sum_q V_q^{\pm} + \sum_{\bar{q}} V_{\bar{q}}^{\pm}, \quad S_{\pm} = \sum_q S_q^{\pm} + \sum_{\bar{q}} S_{\bar{q}}^{\pm}, \qquad (7)$$

where q designates quarks and $\bar{q}$ designates antiquarks. $I_q^-(I_{\bar{q}}^-)$ converts proton (antineutron) quarks into neutron (antiproton) quarks. For example, $I_{\bar{q}}^-(\bar{n}_+) = -\bar{p}_+$. $V_q^-(V_{\bar{q}}^-)$ converts proton (antilambda) quarks into lambda (antiproton) quarks. $S_q^-(S_{\bar{q}}^-)$ lowers the z component of ordinary spin. The singlet (mass splitting) term in the $SU(3)$ octet is $-(\frac{1}{3})^{\frac{1}{2}}(p\bar{p} + n\bar{n} + \lambda\bar{\lambda})$.[8] With these conventions the singlet state which is formed by contraction on $6 \times \bar{6}$ is $-(\frac{1}{6})^{\frac{1}{2}}(p_+\bar{p}_- + n_+\bar{n}_- + \lambda_+\bar{\lambda}_- + p_-\bar{p}_+ + n_-\bar{n}_+ + \lambda_-\bar{\lambda}_+)$. The highest-weight states of other $SU(3) \otimes SU(2)$ representations in a given $SU(6)$ representation are formed by orthogonalizing. The highest-weight state in each N^m

[6] J. Hamermesh, *Group Theory* (Addison-Wesley Publ. Co., Reading, Mass., 1962).

[7] B. Sakita "Argonne National Laboratory Lecture Notes," 1966; R. Delbourgo, M. A. Rashid, A. Salam, and J. Strathdee in *High Energy Physics and Elementary Particles* (International Atomic Energy Agency, Vienna, 1965); S. Pakvasa and S. P. Rosen, Phys. Rev. **147**, 1166 (1966).

[8] D. Horn, Nuovo Cimento **33**, 64 (1964).

TABLE I. The highest-weight $SU(3) \otimes SU(2)$ states of the $SU(6)$ **35** and **70** in quark form. The full **35** and **70** can be generated from these states. $[AB] = AB - BA$.

35	8^3	$p_+\bar{n}_+$
	8^1	$-(\frac{1}{2})^{\frac{1}{2}}(p_+\bar{n}_- + p_-\bar{n}_+)$
	1^3	$-(\frac{1}{3})^{\frac{1}{2}}(p_+\bar{p}_+ + n_+\bar{n}_+ + \lambda_+\bar{\lambda}_+)$
70	8^4	$-(\frac{1}{2})^{\frac{1}{2}}[p_+\lambda_+]p_+$
	10^2	$(\frac{1}{2})^{\frac{1}{2}}[p_+p_-]p_+$
	8^2	$-(\frac{1}{6})^{\frac{1}{2}}\{[p_+\lambda_-]p_+ + [p_-p_+]\lambda_+ + [\lambda_+p_+]p_-\}$
	1^2	$-\frac{1}{6}\{[\lambda_+n_-]p_+ + [p_-\lambda_+]n_+ + [\lambda_-n_+]p_+ + [n_+p_-]\lambda_+ + [p_+\lambda_-]n_+ + [n-p_+]\lambda_+ - 2[n_+p_+]\lambda_- - 2[p_+\lambda_+]n_- - 2[\lambda_+n_+]p_-\}$

representation of the **35** and the **70** is presented in Table I to make our phase conventions clear.

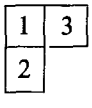
With **35** and **70** in quark notation, it is possible to write any $SU(3) \otimes SU(2)$ product state in quark form, leaving only the multiplet-coupling factors undetermined. Substituting the quark states into Eq. (6):

$$\Phi(1\ \tfrac{5}{2}\ \tfrac{1}{2};\ \tfrac{5}{2}\ \tfrac{1}{2}) = [(\tfrac{1}{3})^{\frac{1}{2}}\alpha]p_+\bar{n}_+[p_+p_-]p_- + [\tfrac{1}{2}\beta - \tfrac{1}{2}(\tfrac{1}{3})^{\frac{1}{2}}\alpha]p_-\bar{n}_+[p_+p_-]p_+ + [\tfrac{1}{2}\beta - \tfrac{1}{2}(\tfrac{1}{3})^{\frac{1}{2}}\alpha]p_+\bar{n}_-[p_+p_-]p_+ . \quad (8)$$

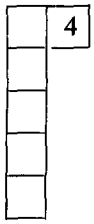
Individual terms in the sum on the right will be referred to as multiquark terms. The convention used here, which is modeled on the convention of Sawada and Yonezawa, is that position in a multiquark term indicates particle number.[9] Thus, in $p_+\bar{\lambda}_+[p_+p_-]p_-$, particle 1 is in state p_+, particle 2 in $\bar{\lambda}_+$, etc. Detailed inspection of the standard tableaux for the various $SU(6)$ product representations yields conditions on α and β which will produce the required symmetry of the irreducible $SU(6)$ representations.

THE USE OF YOUNG DIAGRAMS

To see how this can be done, it is necessary to discuss the standard tableaux of the product states in some detail. For the **70**, we use



For the **35**,



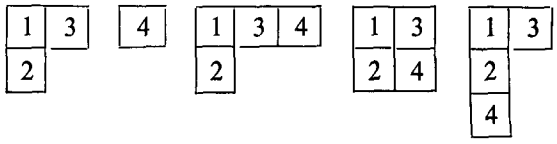
[9] S. Sawada and M. Yonezawa, Progr. Theoret. Phys. (Kyoto) **23**, 662 (1960).

Recall that

$$\mathbf{35} \otimes \mathbf{70} = \mathbf{20} \oplus \mathbf{56} \oplus \mathbf{70} \oplus \mathbf{70} \oplus \mathbf{540} \oplus \mathbf{560} \oplus \mathbf{1134}.$$

It is convenient to consider $\mathbf{35} \otimes \mathbf{70}$ as coming from $\bar{\mathbf{6}} \otimes \mathbf{70} \otimes \mathbf{6}$, since the only term in $\bar{\mathbf{6}} \otimes \mathbf{70} \otimes \mathbf{6}$ which does not belong to $\mathbf{35} \otimes \mathbf{70}$ is $\mathbf{1} \otimes \mathbf{70}$, and that is easily recognized. Now

$$\mathbf{70} \otimes \mathbf{6} = \mathbf{210} \oplus \mathbf{105}_A \oplus \mathbf{105}_B .$$



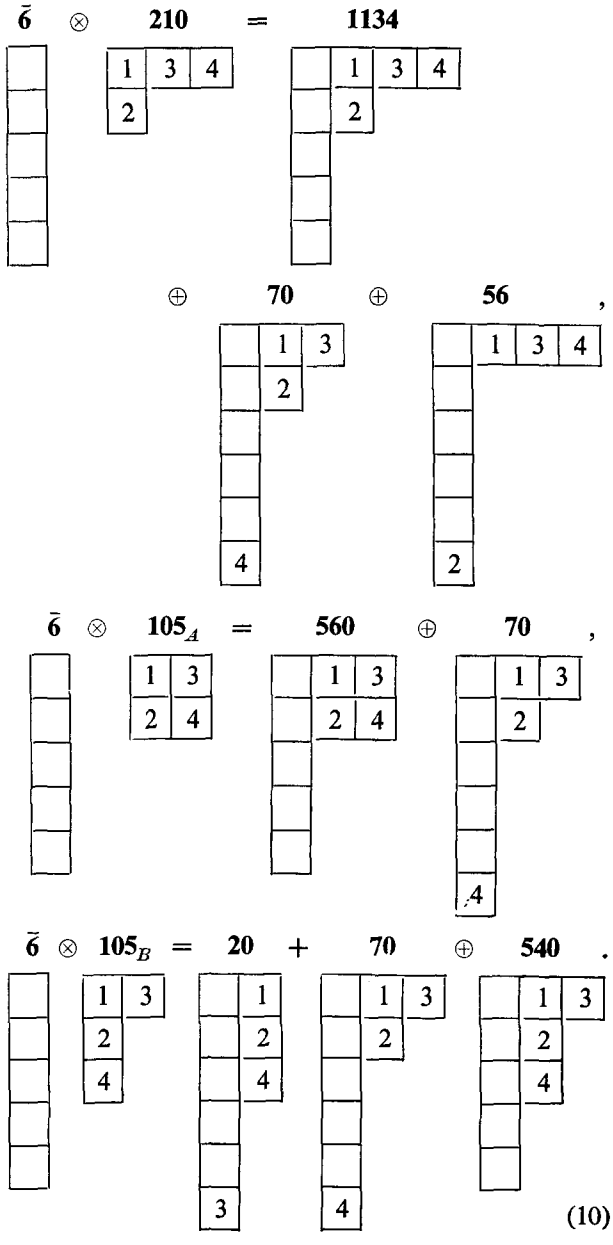
(9)

We now multiply all representations on the right side of (9) by $\bar{\mathbf{6}}$ to get

$$\bar{\mathbf{6}} \otimes \mathbf{210} = \mathbf{1134} \oplus \mathbf{70} \oplus \mathbf{56},$$

$$\bar{\mathbf{6}} \otimes \mathbf{105}_A = \mathbf{560} \oplus \mathbf{70},$$

$$\bar{\mathbf{6}} \otimes \mathbf{105}_B = \mathbf{20} + \mathbf{70} \oplus \mathbf{540}.$$



(10)

We will call $SU(3) \otimes SU(2)$ representations in the product space, which have a higher multiplicity in either $SU(3)$ or $SU(2)$ than either $SU(6)$ parent, the large representations. All other product representations will be called small. For example, 35^2 is a large representation because there is no $SU(3)$ 35 contained in either the **35** or the **70** of the $SU(6)$. It is clear that, for the large representations which can fall only in the **540**, the **560**, or the **1134**, the 4-quark permutation symmetry is unique in every case. For example, in 35^2, the **1134** must have the 4-quark symmetry of the **210**. This immediately makes it possible to reduce Eq. (8). Particles 1 and 4 are symmetrically coupled in the **1134** and antisymmetrically coupled in the **560**. Therefore,

$$(\tfrac{1}{3})^{\frac{1}{2}}\alpha = \tfrac{1}{2}\beta - \tfrac{1}{2}(\tfrac{1}{3})^{\frac{1}{2}}\alpha, \quad \text{for the } \mathbf{1134},$$

and (11)

$$-(\tfrac{1}{3})^{\frac{1}{2}}\alpha = \tfrac{1}{2}\beta - \tfrac{1}{2}(\tfrac{1}{3})^{\frac{1}{2}}\alpha, \quad \text{for the } \mathbf{560}.$$

The addition of the normalization condition determines α and β for both representations. Similar arguments can be used to form all highest-weight states of the large representations. Once the multiplet-coupling coefficients are known, all states of the large representations can be formed. Thus, the state of highest weight in the $SU(3) \otimes SU(2)$ 35^2 of the $SU(6)$ **1134** is

$$\begin{aligned}\Phi_{1134}(1\ \tfrac{5}{2}\ \tfrac{1}{2};\ \tfrac{5}{2}\ \tfrac{1}{2}) = &-\tfrac{1}{2}\Phi_{81}(0\ 1\ 0;\ 1\ 0)\Phi_{10^2}(1\ \tfrac{3}{2}\ \tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2})\\ &+ (\tfrac{3}{4})^{\frac{1}{2}}[(\tfrac{2}{3})^{\frac{1}{2}}\Phi_{83}(0\ 1\ 1;\ 1\ 1)\Phi_{10^2}(1\ \tfrac{3}{2}\ \tfrac{1}{2};\ \tfrac{3}{2}\ -\tfrac{1}{2})\\ &- (\tfrac{1}{3})^{\frac{1}{2}}\Phi_{83}(0\ 1\ 1;\ 1\ 0)\Phi_{10^2}(1\ \tfrac{3}{2}\ \tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2})].\end{aligned}$$

The small N^m representations are formed by contracting the direct product of the parents. The $\mathbf{35} \otimes \mathbf{70}$ contains only one antiquark. In a contracted representation of a $\bar{q}qqqq$ state, the antiquark must be accompanied by its corresponding quark in each multiquark term. A term, therefore, which contains $\bar{\lambda}_+$ must also contain λ_-. This imposes, in general, a number of independent conditions on the multiplet-coupling coefficients. For example, the highest-weight state in the 1^2, when written in the general form of Eq. (8), contains the multiquark term $p_-\bar{\lambda}_+[\lambda_+ n_-]\lambda_+$. The coefficient of this term in both **70**'s must be zero, since there is no λ_- to go with $\bar{\lambda}_+$. Such considerations yield two independent conditions on the multiplet-coupling coefficients, enough to eliminate both large representations.

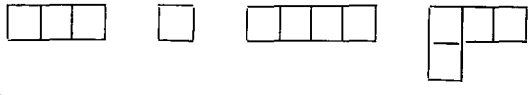
There are cases in which more than one dimensionality results from contracting a product. For example, contracting $\bar{\mathbf{6}} \otimes \mathbf{210}$ gives a **70** and a **56**. The standard tableaux shows that particles 1, 2, and 4 are symmetrically coupled in the **56**. This, in addition to the conditions mentioned earlier, imposes a sufficient number of conditions on the multiplet-coupling coefficients to give a **56**. The orthogonality of the **70** to the **56** can be used to determine the coefficients for the **70**.

THE CLASSIFICATION OF THE TWO 70's

The product $\mathbf{35} \otimes \mathbf{70}$ is not simply reducible. The **70** representation appears twice. In the product $\mathbf{n} \otimes \mathbf{m}$, the permutation symmetry of the parents can be used to classify the products if $\mathbf{n} = \mathbf{m}$. For example, $\mathbf{35} \otimes \mathbf{35} = \mathbf{35}_F \oplus \mathbf{35}_D \oplus \cdots$. If $\mathbf{n} \neq \mathbf{m}$, the case is not so simple. It is, however, possible to make use of the permutation symmetry under quark interchange to classify the products.

One can construct the two **70**'s so that the 4-quark part of one of them contains no **210** symmetry. Since the **1134** comes only from $\bar{\mathbf{6}} \otimes \mathbf{210}$ [cf. Eqs. (10)], this **70** (which we call $\mathbf{70}_{\mathrm{II}}$) cannot be produced by any operation on the $\bar{q}qqqq$ in **1134** states which merely recouples the $\bar{q}$ to the $qqqq$. The W-spin lowering operation is such an operation.[10] We have used this classification (the absence of **210** in $\mathbf{70}_{\mathrm{II}}$) in order to facilitate calculations in which $\mathbf{35} \otimes \mathbf{56} \rightarrow \mathbf{35} \otimes \mathbf{70}$, since the 4-quark permutation symmetry of the **70** in $\mathbf{35} \otimes \mathbf{56}$ must be that of the **210**:

56 $\otimes$ **6** = **126** $\oplus$ **210**



and

$$\bar{\mathbf{6}} \otimes \mathbf{126} = \mathbf{56} \oplus \mathbf{700},$$

$$\bar{\mathbf{6}} \otimes \mathbf{210} = \mathbf{56} \oplus \mathbf{70} \oplus \mathbf{1134}.$$

Where a given $SU(3)^{SU(2)}$ representation occurs more than once in an $SU(6)$ representation (e.g., the 8^4 of **1134**), we have chosen our notation to agree with that of Ref. 1. For example, in the 27^4 of **1134**, two orthogonal 27^4's were found using the techniques described above. Then, the coefficient of the multiquark term involving $\bar{\lambda}_+$ was found by projection. The term of highest S_z, Y, I_z in 27^4 contains $\bar{\lambda}_+\phi(\frac{4}{3}\ 1\ \frac{3}{2};\ 1\ \frac{3}{2})$, where ϕ comes from the 15^3_A of **210**. The scalar product of this term and the highest-weight term of the 27^4 was calculated, and the linear combinations of the 27^4's from $\mathbf{35} \otimes \mathbf{70}$ were adjusted to give the same coefficients of $\bar{\lambda}_+\phi(\frac{4}{3}\ 1\ \frac{3}{2};\ 1\ \frac{3}{2})$ as were

[10] H. Lipkin and S. Meshkov, Phys. Rev. Letters **14**, 670 (1965); H. Harari *et al.*, Phys. Rev. **146**, 1052 (1966).

used in $\mathbf{35} \otimes \mathbf{56}$. The 27^4_A and 27^4_B are thus, in effect, differentiated by their $\bar{\mathbf{6}} \otimes \mathbf{210}$ parentage.

The phases within the product **70**'s have been chosen to agree with those of the parent **70**. The phases within the **56** and the **1134** have been chosen to agree with those previously published for $\mathbf{35} \otimes \mathbf{56}$.[1] [It is to be noted, however, that the conventions used here to generate an $SU(6)$ **35** are different from those of Carter *et al.*[1] This requires that all columns in the tables of Carter, Coyne, and Meshkov[1] which contain an 8^1 or a 1^3 must reverse sign.] This has been checked by use of the $SU(6)$ generator N_-, which lowers the spin of neutron quarks and antiquarks without affecting the other quarks.

The multiplet-coupling coefficients for $\mathbf{35} \otimes \mathbf{70}$ are given in Table II.

ACKNOWLEDGMENTS

The authors are grateful for discussions with D. Horn, M. Kugler, H. Harari, J. Drietlein, L. O'Raifeartaigh, and S. Meshkov.

APPENDIX: PHASES

The phases we have used within the **56** and the **70** have been chosen on the basis of parentage. In $SU(6)$, the **56** comes from $\mathbf{6} \otimes \mathbf{6} \otimes \mathbf{6} = \mathbf{21} \otimes \mathbf{6}$. In $SU(3) \otimes SU(2)$, the **56** comes from $3^2 \otimes 3^2 \otimes 3^2 = [6^3 \oplus \bar{3}^1] \otimes 3^2$. The **70** we have used comes in $SU(6)$ from $\mathbf{6} \otimes \mathbf{6} \otimes \mathbf{6} = \mathbf{15} \otimes \mathbf{6}$. In $SU(3) \otimes SU(2)$, the **70** comes from $3^2 \otimes 3^2 \otimes 3^2 = [6^1 \oplus \bar{3}^3] \otimes 3^2$. To select the overall phase of an $SU(3) \otimes SU(2)$ multiplet within the **56** or the **70**, we have first written out the highest weight state in each multiplet. A plus sign is then given to that term which contains the highest-weight contribution from the $SU(6)$ **21** or **15**. The highest-weight state in 6^3 is p_+p_+; in 3^1,

$$\tfrac{1}{2}[p_+\lambda_- - p_-\lambda_+ + \lambda_-p_+ - \lambda_+p_-];$$

in 6^1, $(\frac{1}{2})^{\frac{1}{2}}[p_+p_-]$; in $\bar{3}^3$, $(\frac{1}{2})^{\frac{1}{2}}[p_+\lambda_+]$. In the **56**, the $SU(3) \otimes SU(2)$ parents are $10^4 = (6^3 \otimes 3^2)$ and $8^2 = (6^3 \otimes 3^2)$. In the **70**, they are $8^4 = (\bar{3}^3 \otimes 3^2)$; $10^2 = (6^1 \otimes 3^2)$; $8^2 = [(\frac{1}{2})^{\frac{1}{2}}(6^1 \otimes 3^2) + (\frac{1}{2})^{\frac{1}{2}}(\bar{3}^3 \otimes 3^2)]$; and $1^2 = (\bar{3}^3 \otimes 3^2)$.

TABLE II. $SU(6)$ Clebsch–Gordan coefficients for the product $\mathbf{35} \otimes \mathbf{70}$. The columns are the representations of $SU(6)$ and the rows are their $SU(3) \otimes SU(2)$ components. Each number is to be divided by the normalization at the bottom of its column.

27^6

	1134
$(8^3 \times 8^4)$	-1

$\overline{10}^6$

	560
$(8^3 \times 8^4)$	-1

10^6

	1134
$(8^3 \times 8^4)$	1

8^6

	540	560	1134
$(8^3 \times 8^4)_S$	$-\sqrt{5}$	$-\sqrt{5}$	$+1$
$(8^3 \times 8^4)_A$	-3	1	$-\sqrt{5}$
$(1^3 \times 8^4)$	$-\sqrt{2}$	$\sqrt{2}$	$+\sqrt{10}$
N	4	$2\sqrt{2}$	4

1^6

	540
$(8^3 \times 8^4)$	-1

35^4

	1134
$(8^3 \times 10^2)$	1

27^4

	540	560	1134_A	1134_B
$(8^3 \times 8^4)$	$-\sqrt{5}$	$\sqrt{5}$	$-\sqrt{3}$	$\sqrt{5}$
$(8^3 \times 10^2)$	$2\sqrt{2}$	$2\sqrt{2}$	0	$2\sqrt{2}$
$(8^3 \times 8^2)$	0	$2\sqrt{2}$	0	$-4\sqrt{2}$
$(8^1 \times 8^4)$	$-\sqrt{3}$	$\sqrt{3}$	$\sqrt{5}$	$\sqrt{3}$
N	4	$2\sqrt{6}$	$2\sqrt{2}$	$4\sqrt{3}$

10^4

	56	540	560	1134_A	1134_B
$(8^3 \times 8^4)$	$-\sqrt{5}$	$\sqrt{5}$	$-\sqrt{5}$	-3	$-\sqrt{5}$
$(8^3 \times 10^2)$	2	2	2	$-2\sqrt{5}$	2
$(8^3 \times 8^2)$	$\sqrt{2}$	0	$-2\sqrt{2}$	0	$16\sqrt{2}$
$(8^1 \times 8^4)$	$\sqrt{3}$	$\sqrt{3}$	$-\sqrt{3}$	$\sqrt{15}$	$-9\sqrt{3}$
$(1^3 \times 10^2)$	-1	2	2	$2\sqrt{5}$	14
N	$\sqrt{15}$	4	$2\sqrt{6}$	8	$8\sqrt{15}$

$\overline{10}^4$

	540	560	1134
$(8^3 \times 8^4)$	$-\sqrt{5}$	$-\sqrt{3}$	$\sqrt{5}$
$(8^3 \times 8^2)$	$2\sqrt{2}$	0	$2\sqrt{2}$
$(8^1 \times 8^4)$	$-\sqrt{3}$	$\sqrt{5}$	$\sqrt{3}$
N	4	$2\sqrt{2}$	4

1^4

	20	540	560	1134
$(8^3 \times 8^4)$	$-\sqrt{10}$	-1	$-\sqrt{5}$	$-\sqrt{5}$
$(8^3 \times 8^2)$	-2	$4\sqrt{10}$	$2\sqrt{2}$	0
$(8^1 \times 8^4)$	$\sqrt{6}$	$3\sqrt{15}$	$-\sqrt{3}$	$-\sqrt{3}$
$(1^3 \times 1^2)$	-1	$2\sqrt{10}$	$-2\sqrt{2}$	$2\sqrt{2}$
N	$\sqrt{21}$	$4\sqrt{21}$	$2\sqrt{6}$	4

8^4

	70_I	70_{II}	540_A	540_B	540_C	560_A	560_B	1134_A	1134_B	1134_C
$(8^3 \times 8^4)_S$	-5	15	0	$5\sqrt{2}$	5	0	$-\sqrt{5}$	-5	-3	$-\sqrt{5}$
$(8^3 \times 8^4)_A$	$5\sqrt{5}$	$\sqrt{5}$	$-3\sqrt{10}$	0	$-\sqrt{5}$	$\sqrt{2}$	-3	$-\sqrt{5}$	$3\sqrt{5}$	5
$(8^3 \times 10^2)$	$-\sqrt{10}$	$-5\sqrt{10}$	$\sqrt{5}$	$3\sqrt{5}$	$-\sqrt{10}$	-1	$-3\sqrt{2}$	0	$\sqrt{10}$	$7\sqrt{2}$
$(8^3 \times 8^2)_S$	$-2\sqrt{10}$	$-2\sqrt{10}$	$-5\sqrt{5}$	$-\sqrt{5}$	0	-1	$2\sqrt{2}$	$-\sqrt{10}$	$-2\sqrt{10}$	$6\sqrt{2}$
$(8^3 \times 8^2)_A$	$4\sqrt{2}$	$-4\sqrt{2}$	-5	3	$10\sqrt{2}$	$-\sqrt{5}$	0	$\sqrt{2}$	0	$-4\sqrt{10}$
$(8^3 \times 1^2)$	$3\sqrt{2}$	$-\sqrt{2}$	5	-1	$-5\sqrt{2}$	$-\sqrt{5}$	$\sqrt{10}$	$-4\sqrt{2}$	$5\sqrt{2}$	$-\sqrt{10}$
$(8^1 \times 8^4)_S$	$\sqrt{15}$	$-3\sqrt{15}$	$\sqrt{30}$	0	$3\sqrt{15}$	$\sqrt{6}$	$\sqrt{3}$	$-\sqrt{15}$	$-\sqrt{15}$	$\sqrt{3}$
$(8^1 \times 8^4)_A$	$-5\sqrt{3}$	$-\sqrt{3}$	0	$-3\sqrt{6}$	$5\sqrt{3}$	0	$-\sqrt{15}$	$-\sqrt{3}$	$5\sqrt{3}$	$-\sqrt{15}$
$(1^3 \times 8^4)$	$-2\sqrt{10}$	$-2\sqrt{10}$	$-2\sqrt{5}$	$2\sqrt{5}$	$-2\sqrt{10}$	2	$2\sqrt{2}$	0	$2\sqrt{10}$	$-10\sqrt{2}$
$(1^3 \times 8^2)$	-2	6	0	$2\sqrt{2}$	10	0	$2\sqrt{5}$	2	10	$6\sqrt{5}$
N	$8\sqrt{6}$	$16\sqrt{3}$	$8\sqrt{5}$	$8\sqrt{3}$	$8\sqrt{10}$	$2\sqrt{6}$	$4\sqrt{6}$	$4\sqrt{6}$	$8\sqrt{6}$	$16\sqrt{3}$

35^2

	560	1134
$(8^3 \times 10^2)$	$\sqrt{3}$	-1
$(8^1 \times 10^2)$	1	$\sqrt{3}$
N	2	2

27^2

	540_A	540_B	560	1134_A	1134_B
$(8^3 \times 8^4)$	0	-2	2	0	2
$(8^3 \times 10^2)$	$\sqrt{3}$	1	1	$-\sqrt{3}$	1
$(8^3 \times 8^2)$	$-\sqrt{3}$	0	1	$-\sqrt{3}$	-2
$(8^1 \times 10^2)$	1	$-\sqrt{3}$	$-\sqrt{3}$	-1	$-\sqrt{3}$
$(8^1 \times 8^2)$	-1	0	$-\sqrt{3}$	-1	$2\sqrt{3}$
N	$2\sqrt{2}$	$2\sqrt{2}$	$2\sqrt{3}$	$2\sqrt{2}$	$2\sqrt{6}$

10^2

	70_I	70_{II}	540	560	1134_A	1134_B
$(8^3 \times 8^4)$	2	-10	2	2	-2	-2
$(8^3 \times 10^2)$	$-4\sqrt{2}$	$4\sqrt{2}$	$2\sqrt{2}$	$\sqrt{2}$	0	$2\sqrt{2}$
$(8^3 \times 8^2)$	5	1	3	1	5	-1
$(8^1 \times 10^2)$	$2\sqrt{6}$	$2\sqrt{6}$	0	$\sqrt{6}$	$-2\sqrt{6}$	0
$(8^1 \times 8^2)$	$-\sqrt{3}$	$3\sqrt{3}$	$\sqrt{3}$	$-\sqrt{3}$	$-\sqrt{3}$	$-3\sqrt{3}$
$(1^3 \times 10^2)$	$2\sqrt{2}$	$-2\sqrt{2}$	$2\sqrt{2}$	$-2\sqrt{2}$	$-2\sqrt{2}$	$2\sqrt{2}$
N	$4\sqrt{6}$	$8\sqrt{3}$	$4\sqrt{2}$	$2\sqrt{6}$	8	$4\sqrt{3}$

$\overline{10^2}$

	540	560	1134
$(8^3 \times 8^4)$	-2	0	2
$(8^3 \times 8^2)$	1	$\sqrt{3}$	-1
$(8^1 \times 8^2)$	$-\sqrt{3}$	1	$\sqrt{3}$
N	$2\sqrt{2}$	2	$2\sqrt{2}$

1^2

	70_I	70_{II}	540	1134
$(8^3 \times 8^4)$	$2\sqrt{3}$	-2	-2	-2
$(8^3 \times 8^2)$	$\sqrt{3}$	7	1	3
$(8^1 \times 8^2)$	1	$-3\sqrt{3}$	$3\sqrt{3}$	$\sqrt{3}$
$(1^3 \times 1^2)$	0	-4	-4	4
N	4	$4\sqrt{6}$	$4\sqrt{3}$	$4\sqrt{2}$

8^2

	20	56	70_I	70_{II}	540_A	540_B	540_C	560_A	560_B	1134_A	1134_B	1134_C
$(8^3 \times 8^4)_S$	$2\sqrt{5}$	$2\sqrt{5}$	$-4\sqrt{5}$	$-4\sqrt{5}$	$-2\sqrt{5}$	$-4\sqrt{5}$	$-\sqrt{5}$	$4\sqrt{5}$	$\sqrt{5}$	$8\sqrt{5}$	-6	4
$(8^3 \times 8^4)_A$	-6	2	8	-8	-10	0	1	0	3	-4	$-6\sqrt{5}$	$8\sqrt{5}$
$(8^3 \times 10^2)$	$3\sqrt{5}$	$-\sqrt{5}$	$5\sqrt{5}$	$\sqrt{5}$	$-5\sqrt{5}$	$3\sqrt{5}$	0	$-3\sqrt{5}$	0	$9\sqrt{5}$	-1	-1
$(8^3 \times 8^2)_S$	$-\sqrt{5}$	$\sqrt{5}$	$-2\sqrt{5}$	$6\sqrt{5}$	$-4\sqrt{5}$	$14\sqrt{5}$	$-\sqrt{5}$	$-8\sqrt{5}$	$\sqrt{5}$	$2\sqrt{5}$	8	18
$(8^3 \times 8^2)_A$	-3	-5	-2	-10	0	30	-5	0	-3	10	0	$10\sqrt{5}$
$(8^3 \times 1^2)$	-1	3	3	7	5	5	-6	-5	-2	-1	$-7\sqrt{5}$	$11\sqrt{5}$
$(8^1 \times 10^2)$	$-\sqrt{15}$	$-\sqrt{15}$	$-\sqrt{15}$	$3\sqrt{15}$	$-3\sqrt{15}$	$-15\sqrt{15}$	0	$3\sqrt{15}$	0	$3\sqrt{15}$	$-3\sqrt{3}$	$-3\sqrt{3}$
$(8^1 \times 8^2)_S$	$\sqrt{15}$	$-\sqrt{15}$	0	0	$2\sqrt{15}$	$-12\sqrt{15}$	$-\sqrt{15}$	$-2\sqrt{15}$	$\sqrt{15}$	$-4\sqrt{15}$	$-2\sqrt{3}$	$8\sqrt{3}$
$(8^1 \times 8^2)_A$	$-\sqrt{3}$	$\sqrt{3}$	$4\sqrt{3}$	$4\sqrt{3}$	$10\sqrt{3}$	0	$-\sqrt{3}$	$10\sqrt{3}$	$\sqrt{3}$	$8\sqrt{3}$	$2\sqrt{15}$	$4\sqrt{15}$
$(8^1 \times 1^2)$	$-\sqrt{3}$	$-\sqrt{3}$	$\sqrt{3}$	$-3\sqrt{3}$	$-5\sqrt{3}$	$15\sqrt{3}$	$-2\sqrt{3}$	$5\sqrt{3}$	$2\sqrt{3}$	$-3\sqrt{3}$	$3\sqrt{15}$	$-9\sqrt{15}$
$(1^3 \times 8^4)$	$2\sqrt{2}$	$-2\sqrt{2}$	$-2\sqrt{2}$	$6\sqrt{2}$	0	$50\sqrt{2}$	$\sqrt{2}$	$10\sqrt{2}$	$\sqrt{2}$	$-6\sqrt{2}$	$-4\sqrt{10}$	$2\sqrt{10}$
$(1^3 \times 8^2)$	$2\sqrt{2}$	$2\sqrt{2}$	$2\sqrt{2}$	$2\sqrt{2}$	$-10\sqrt{2}$	$-10\sqrt{2}$	$-2\sqrt{2}$	$10\sqrt{2}$	$-2\sqrt{2}$	$-14\sqrt{2}$	$2\sqrt{10}$	$6\sqrt{10}$
N	$2\sqrt{42}$	$2\sqrt{30}$	$8\sqrt{6}$	$16\sqrt{3}$	$4\sqrt{70}$	$8\sqrt{210}$	$4\sqrt{7}$	$12\sqrt{10}$	$6\sqrt{2}$	$8\sqrt{30}$	$8\sqrt{15}$	$16\sqrt{15}$

F Model on a Triangular Lattice

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(Received 24 February 1969)

The Rys F model is formulated on a triangular lattice and solved for certain values of the vertex configuration probabilities (including those corresponding to the "ice model"). As with the square lattice, it is found that the system undergoes a phase transition which is of infinite order.

1. INTRODUCTION

Lieb[1] has recently solved the ice model, the F model of Rys,[2] and the Slater KDP model for a plane square lattice. These models reduce to counting the number of ways of placing arrows on the bonds of the lattice such that there are as many arrows pointing in to each vertex as there are pointing out, and such that there are given numbers of the various allowed types of vertices.

Clearly such models can be formulated on any lattice with an even number of neighbors per site and, in particular, one might be tempted to think that for a triangular lattice the solutions could be obtained by a straightforward extension of Lieb's work. It turns out, however, that there are difficulties.

In this paper we formulate the F model on a plane triangular lattice and find that the most obvious ansatz for the solution works only when a restriction is imposed on the probabilities of the various types of vertices. Nevertheless, this case is still of some interest, since it includes the triangular "ice model" and predicts an infinite-order phase transition similar to that found for the square lattice.

2. PARTITION FUNCTION AND TRANSFER MATRIX

Suppose that arrows are placed on the bonds of a triangular lattice so that there are three entering and leaving each site or vertex. There are then 20 possible configurations of arrows at each vertex, and if any configurations which can be obtained from one another by rotation or reflection are given equal weight, they can be classified as follows: (i) 6 vertices in which the three incoming arrows are adjacent, (ii) 2 vertices in which the incoming and outgoing arrows alternate round the vertex, (iii) 12 other vertices. Examples of each of these three types are shown in Fig. 1.

If we assign interaction energies ϵ_1, ϵ_2, ϵ_3, respectively, to these three types of vertex, then the problem becomes the calculation of the partition function

$$Z = \sum a^p b^q c^r I(p, q, r), \tag{1}$$

where $a = \exp(-\epsilon_1/kT)$, $b = \exp(-\epsilon_2/kT)$, $c = \exp(-\epsilon_3/kT)$ (k being Boltzmann's constant and T the temperature), and $I(p, q, r)$ is the number of allowed ways of arranging arrows on the lattice so that there are p vertices of type (i), q of type (ii), and r of type (iii).

With any lattice problem we have a choice of possible boundary conditions that can be imposed. In this case we prefer to use a helical boundary condition in which the right-hand site of a row is considered to be the same as the left-hand site of the row above, since this rather simplifies the subsequent transfer-matrix and eigenvalue equations.

We can, therefore, consider a triangular lattice with N sites per row and a total number of sites L, such that the sites can be ordered from left to right and upwards as indicated in Fig. 2. Further, parameters $\alpha_1, \cdots, \alpha_{2L}$, $\beta_1, \cdots, \beta_L$ can be associated with the bonds of the lattice as in Fig. 2, such that α_i (β_i) is zero if the arrow on the corresponding bond points upwards (to the right) and is unity if the arrow points downwards (to the left).

The configurations of the arrows at the vertex i is then specified by the six parameters β_{i-1}, β_i, α_{2i-2N}, $\alpha_{2i-2N+1}$, α_{2i-1}, α_{2i} and the condition that there be three incoming and three outgoing arrows can be seen to imply that

$$\beta_i + \beta_{2i-1} + \alpha_{2i} = \beta_{i-1} + \alpha_{2i-2N+1} + \alpha_{2i-2N}. \tag{2}$$

Imposing cyclic end conditions on the helix, so that $\alpha_{i-2L} = \alpha_i$, $\beta_{i-L} = \beta_i$, the partition function (1)

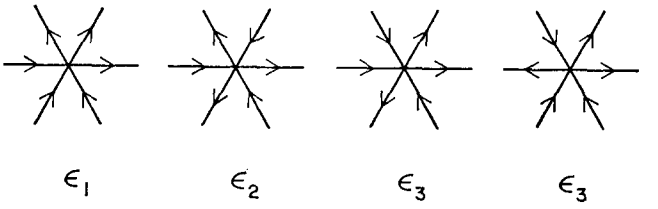

FIG. 1. Examples of the three types of allowed vertex with corresponding interaction energies.

[1] E. H. Lieb, Phys. Rev. Letters **18**, 692 (1967); **18**, 1046 (1967); **19**, 108 (1967); Phys. Rev. **162**, 162 (1967).
[2] F. Rys, Helv. Phys. Acta **36**, 537 (1963).

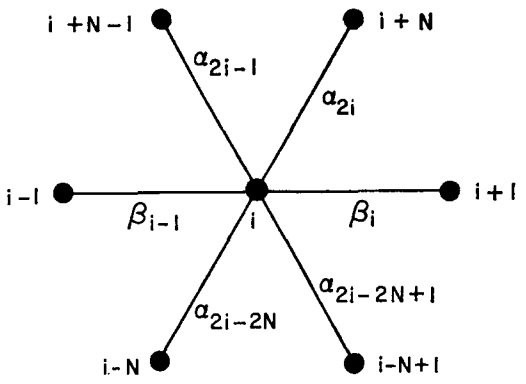

FIG. 2. The labeling of sites and bond parameters.

can be written as

$$Z_L = \sum \prod_{i=1}^{L} K(\beta_i, \alpha_{2i-1}, \alpha_{2i}, \beta_{i-1}, \alpha_{2i-2N+1}, \alpha_{2i-2N}), \tag{3}$$

where the summation is over all values (0 or 1) of the α's and β's, and the function K ensures the correct contribution of each vertex, i.e., K vanishes if the condition (2) is violated, else assumes the values a, b, or c,according as the vertex is of type (i), (ii), or (iii).

Setting $M = 2N - 1$ and defining a 2^{2N} by 2^{2N} matrix V with elements

$$V_{\beta,\alpha_1,\cdots,\alpha_M|\beta',\alpha_1',\cdots,\alpha_M'} = K(\beta, \alpha_{M-1}, \alpha_M, \beta', \alpha_2', \alpha_1')\delta_{\alpha_1\alpha_3'}\delta_{\alpha_2\alpha_4'}\cdots\delta_{\alpha_{M-2},\alpha_M'}, \tag{4}$$

Eq. (3) can be written very simply as

$$Z_L = \mathrm{Tr}\, \mathsf{V}^L. \tag{5}$$

Thus, when L becomes large,

$$Z_L \sim \lambda^L, \tag{6}$$

where λ is the greatest eigenvalue of the matrix V. Writing the corresponding eigenvector as

$$h_\beta(\alpha_1, \cdots, \alpha_M),$$

it follows from (4) that λ is given by

$$\lambda h_\beta(\alpha_1, \cdots, \alpha_M) = \sum_{\beta',\alpha''} K(\beta, \alpha_{M-1}, \alpha_M, \beta', \alpha'', \alpha') \times h_{\beta'}(\alpha', \alpha'', \alpha_1, \cdots, \alpha_{M-2}). \tag{7}$$

Since K vanishes unless its arguments in (3) satisfy the condition (2), the eigenvalue equation (7) has the important property that the number $\beta + \alpha_1 + \cdots + \alpha_M$ is conserved. Thus, one can look for an eigenvector $h_\beta(\alpha_1, \cdots, \alpha_M)$ whose elements are zero unless

$$\beta + \alpha_1 + \cdots + \alpha_M = n, \tag{8}$$

where n can assume the values $0, 1, \cdots, 2N$. When N is large, the ratio

$$n/N = 1 - y \tag{9}$$

is the ratio of down arrows to up arrows in each row of the lattice.

The nonzero elements of $h_0(\alpha_1, \cdots, \alpha_M)$ must have exactly n α's equal to one, the rest being zero. For these elements one can therefore write

$$h_0(\alpha_1, \cdots, \alpha_M) = f_{j_1,\cdots,j_n}, \tag{10a}$$

where $j_1, \cdots, j_n$ are the values of i for which $\alpha_i = 1$. Clearly these can be ordered so that $1 \leqslant j_1 < j_2 < \cdots < j_n \leqslant M$. Similarly, one can write

$$h_1(\alpha_1, \cdots, \alpha_M) = g_{j_1,\cdots,j_{n-1}}, \tag{10b}$$

where $1 \leqslant j_1 < \cdots < j_{n-1} \leqslant M$.

Substituting the forms (10) of the nonzero elements of $h_\beta(\alpha_1, \cdots, \alpha_M)$ into Eq. (7), writing the values of the function K—namely 0, a, b, or c—explicitly in the appropriate terms, and for convenience replacing each j_m by $j_m - 2$, one obtains the set of equations

$$\lambda f_{j_1-2,\cdots,j_n-2} = a f_{j_1,\cdots,j_n}, \tag{11a}$$

$$\begin{aligned}
\lambda f_{j_1-2,\cdots,j_{n-1}-2,M} &= b f_{1,j_1,\cdots,j_{n-1}} + c g_{j_1,\cdots,j_{n-1}} \\
&\quad + c f_{2,j_1,\cdots,j_{n-1}}, \\
\lambda g_{j_1-2,\cdots,j_{n-1}-2} &= c f_{1,j_1,\cdots,j_{n-1}} + a g_{j_1,\cdots,j_{n-1}} \\
&\quad + c f_{2,j_1,\cdots,j_{n-1}}, \\
\lambda f_{j_1-2,\cdots,j_{n-1}-2,M-1} &= c f_{1,j_1,\cdots,j_{n-1}} + c g_{j_1,\cdots,j_{n-1}} \\
&\quad + a f_{2,j_1,\cdots,j_{n-1}},
\end{aligned} \tag{11b}$$

$$\begin{aligned}
\lambda g_{j_1-2,\cdots,j_{n-2}-2,M-1} &= b g_{2,j_1,\cdots,j_{n-2}} + c f_{1,2,j_1,\cdots,j_{n-2}} \\
&\quad + c g_{1,j_1,\cdots,j_{n-2}}, \\
\lambda f_{j_1-2,\cdots,j_{n-2}-2,M-1,M} &= c g_{2,j_1,\cdots,j_{n-2}} + a f_{1,2,j_1,\cdots,j_{n-2}} \\
&\quad + c g_{1,j_1,\cdots,j_{n-2}}, \\
\lambda g_{j_1-2,\cdots,j_{n-2}-2,M} &= c g_{2,j_1,\cdots,j_{n-2}} + c f_{1,2,j_1,\cdots,j_{n-2}} \\
&\quad + a g_{1,j_1,\cdots,j_{n-2}},
\end{aligned} \tag{11c}$$

$$\lambda g_{j_1-2,\cdots,j_{n-3}-2,M-1,M} = a g_{1,2,j_1,\cdots,j_{n-3}}, \tag{11d}$$

where the j's in each equation lie in the range $3 \leqslant j_1 < j_2 < \cdots \leqslant M$.

3. APPLICATION OF THE ANSATZ

We now attempt to solve the eigenvalue equations (11) by assuming a form for the eigenvector. For the square lattice the appropriate ansatz is a sum of plane waves,[1] but for the present model we have to differentiate between the j's being odd and even, due to the fact that these correspond to down arrows on different types of diagonal bonds. It turns out that the most elementary extension of the plane-wave

ansatz that can possibly satisfy (11) is

$$f_{j_1,\cdots,j_n} = \sum A_{m_1,\cdots,m_n}\phi_{m_1}(j_1)\cdots\phi_{m_n}(j_n),$$
$$g_{j_1,\cdots,j_{n-1}} = \sum A_{m_1,\cdots,m_n}V_{m_1}\phi_{m_2}(j_1)\cdots\phi_{m_n}(j_{n-1}), \tag{12}$$

where $\{m_1,\cdots,m_n\}$ is any permutation of the numbers $\{1,\cdots,n\}$ and the summations are over all such permutations. The functions $\phi_m(j)$ are defined by

$$\phi_m(j) = U_m X_m^{\frac{1}{2}(j-1)}, \quad \text{if } j \text{ is odd},$$
$$= W_m X_m^{\frac{1}{2}(j-2)}, \quad \text{if } j \text{ is even}, \tag{13}$$

where $m = 1,\cdots,n$.

We now try to choose the variables in (12) and (13) so as to satisfy (11). We first note that (11a) is satisfied if

$$\lambda = aX_1X_2\cdots X_n. \tag{14}$$

Using this result and remembering that $M = 2N-1$, the three equations (11b) are satisfied if there exists a set of quantities $Y_1,\cdots,Y_n$ such that

$$A_{m_2,\cdots,m_n,m_1} = X_{m_1}^{1-N}Y_{m_1}A_{m_1,m_2,\cdots,m_n}, \tag{15}$$

where, for any m in the range $1 \leqslant m \leqslant n$, U_m, V_m, W_m, X_m, and Y_m are related by the matrix equation

$$\begin{pmatrix} aX_mY_m - b & -c & -c \\ -c & aX_m - a & -c \\ -c & -c & aY_m - a \end{pmatrix}\begin{pmatrix} U_m \\ V_m \\ W_m \end{pmatrix} = \mathbf{0}. \tag{16}$$

Using (14) and (15) and applying the ansatz to the three equations (11c), it is found that they are satisfied if

$$s^{(p)}_{m_1,m_2}A_{m_1,m_2,m_3,\cdots,m_n} + s^{(p)}_{m_2,m_1}A_{m_2,m_1,m_3,\cdots,m_n} = 0 \tag{17}$$

for $p = 1, 2, 3$, where

$$\begin{aligned} s^{(1)}_{m,m'} &= aY_mW_mX_{m'}V_{m'} - bV_mW_{m'} \\ &\quad - cU_mW_{m'} - cV_mU_{m'}, \\ s^{(2)}_{m,m'} &= aY_mW_mX_{m'}Y_{m'}U_{m'} \\ &\quad - cV_mW_{m'} - aU_mW_{m'} - cV_mU_{m'}, \\ s^{(3)}_{m,m'} &= aX_mY_mU_mX_{m'}V_{m'} - cV_mW_{m'} \\ &\quad - cU_mW_{m'} - aV_mU_{m'}. \end{aligned} \tag{18}$$

Similarly, (11d) leads to the condition

$$\sum [Y_mW_mX_{m'}Y_{m'}U_{m'}X_{m''}V_{m''} - V_mU_{m'}W_{m''}]A_{m,m',m'',m_4,\cdots,m_n} = 0, \tag{19}$$

where the summation is over all six permutations $\{m, m', m''\}$ of the numbers m_1, m_2, m_3.

4. SOLUTION OF THE ANSATZ EQUATIONS

If we can solve Eqs. (14)–(19), then we have a solution of the eigenvalue equations (11). First note that (15) relates two A's which differ by a cyclic shift of the suffixes $m_1,\cdots,m_n$. Performing such a shift n times, therefore, leads to the condition

$$\prod_{m=1}^{n} X_m^{1-N}Y_m = 1, \tag{20}$$

$X_1,\cdots,X_n$ can be eliminated from Eqs. (14) and (20) to give an alternative expression for λ, namely,

$$(\lambda/a)^{N-1} = Y_1Y_2\cdots Y_n. \tag{21}$$

For (16) to be satisfied nontrivially, the determinant of the 3 by 3 matrix must vanish, giving a relation between X_m and Y_m. The ratios $U_m:V_m:W_m$ can then be calculated in terms of X_m and Y_m.

It is at the three equations (17) that the major stumbling block to the ansatz occurs, for in order for these to be satisfied nontrivially the ratio $s^{(p)}_{m,m'}/s^{(p)}_{m',m}$ must be the same for all three values of p. In general, it appears to be impossible to satisfy this condition.

Some rather startling simplifications occur, however, when the vertex weights a, b, c satisfy the relation

$$(a-c)^2 = a(b-c). \tag{22}$$

(Note in particular that this includes the "triangular ice model," where a, b, c are equal.) In this case the solutions of the determinantal relation between X_m and Y_m implied by (16) can be parametrized as rational functions of a third variable z_m. It turns out that the most convenient way of doing this is to first introduce a variable w such that

$$c/a = 1 + w + w^{-1}. \tag{23}$$

Using (22), z_m can then be defined so that the solutions of (16) are

$$X_m = \frac{1-w^2z_m}{w^2-z_m}\cdot\frac{1-wz_m}{w-z_m}, \tag{24}$$

$$Y_m = w^{-2}\frac{z_m-w^2}{1-z_m}\cdot\frac{z_m-w^3}{1-wz_m}, \tag{25}$$

$$U_m:V_m:W_m = 1:\frac{w^{-1}z_m-w}{1-z_m}:\frac{1-wz_m}{z_m-w}. \tag{26}$$

Substituting the expressions (24)–(26) into the equations (18) and using (22) and (23), one obtains the unexpected but welcome result that

$$\frac{s^{(p)}_{m,m'}}{s^{(p)}_{m',m}} = \frac{z_m-w^3z_{m'}}{z_{m'}-w^3z_m} \tag{27}$$

for $p = 1, 2, 3$. Thus this ratio is indeed independent of p and (17) now represents one equation, rather than three. Further, making the same substitutions in Eq. (19) and using (15) and (17), it is found (after a very tedious calculation) that the equation is satisfied identically for any values of the z_m.

It therefore remains to solve Eqs. (15) and (17). This can be done, provided only that

$$X_m Y_m X_m^{-N} = -\prod_{m'=1}^{n}\left\{-\frac{z_m - w^3 z_{m'}}{z_{m'} - w^3 z_m}\right\} \tag{28}$$

for $m = 1, \cdots, n$. Thus the ansatz does in fact work when the restriction (22) is imposed on a, b, and c, for in principle $z_1, \cdots, z_n$ can be chosen to ensure that the n conditions (28) are satisfied. Equation (14) or, equivalently, (21), then gives the eigenvalue λ.

5. SOLUTION FOR LARGE N

The problem now is to solve Eq. (28), together with (24) and (25), for $z_1, \cdots, z_n$. In particular, we are interested in the limit when n and N become large, the ratio (9) being kept constant.

We would like to apply reasoning similar to that used by Yang[3] for the Heisenberg chain, and by Lieb[1] for the square lattice models. An obstacle to this is the term $X_m Y_m$ on the left-hand side of Eq. (28) which arises from the helical boundary condition. However, the other terms in the equation depend exponentially on N and n, so that the contribution of the factor $X_m Y_m$ may be expected to be negligible in the limit when these are large. More specifically, the error introduced in $z_1, \cdots, z_n$ by neglecting $X_m Y_m$ should be of order N^{-1}, except for a relatively small number (of order $\log N$) of parameters such that $z_m \simeq 1$ and for which $Y_m \sim N$. The author has not been able to prove these assertions in general, but they are certainly true for the special case $c = 2a$.

It must be noted that such errors will be significant in Eq. (14), leading to a finite error in λ. However, the situation can be saved by instead calculating λ from Eq. (21), for which such errors will be negligible.

Neglecting therefore the term $X_m Y_m$, re-arranging slightly, and using (24), Eq. (28) can be written as

$$R(z_m) = (-)^{n-1}, \tag{29}$$

where the function $R(z)$, which depends implicitly on $z_1, \cdots, z_n$, is defined by

$$R(z) = \left\{\frac{1 - wz}{w - z}\,\frac{1 - w^2 z}{w^2 - z}\right\}^N \prod_{m'=1}^{n}\left\{\frac{z - w^3 z_{m'}}{z_{m'} - w^3 z}\right\}. \tag{30}$$

Inspection of these equations reveals that a solution can be chosen so that to any z_m there corresponds a $z_{m'}$ such that $z_{m'} = z_m^{-1}$. In particular, this implies that $R(1) = 1$. The solution of (29) which maximizes λ can then be obtained by taking the logarithm of both sides so that

$$\log R(z_m) = i\pi(2m - n - 1), \tag{31}$$

for $m = 1, \cdots, n$, where the branch of the logarithm on the left-hand side is chosen so that $\log R(1) = 0$. This ordering ensures that $z_{n+1-m} = z_m^{-1}$.

It is apparent from (23) that w lies on the unit circle if $c < 3a$, while it is real and positive if $c > 3a$. These two cases will be considered separately in the next sections.

6. THE CASE $c < 3a$

In this case, w can be chosen to be

$$w = \exp(-i\phi), \tag{32}$$

where $0 < \phi < \frac{2}{3}\pi$ (the upper bound is required by the condition that c and a be positive). The variables $z_1, \cdots, z_n$ are then real and positive, so that one can set

$$z_m = \exp(u_m), \tag{33}$$

where $u_{n+1-m} = -u_m$.

Define a function

$$F(\theta, u) = \pi^{-1} \tan^{-1}\{\cot \tfrac{1}{2}\theta \tanh \tfrac{1}{2}u\} \tag{34}$$

such that $F(\theta, u)$ is a continuous function of u for $-\infty < u < \infty$ and is zero when $u = 0$. Then, using the form (30) of $R(z)$, Eq. (31) becomes

$$\tfrac{1}{2}(2m - n - 1) = NF(\phi, u_m) + NF(2\phi, u_m) - \sum_{m'=1}^{n} F(3\phi, u_m - u_{m'}). \tag{35}$$

As n and N become large, the ratio (9) being held fixed at some value not greater than one, the u_m's tend to a continuous distribution in some range $(-Q, Q)$ such that $-Q < u_1 < \cdots < u_n < Q$. If $N\rho(u)\,du$ is the number of u_m's in the interval $(u, u + du)$, then Eq. (35) becomes in the limit

$$\int_0^u \rho(u')\,du' = F(\phi, u) + F(2\phi, u) - \int_{-Q}^{Q} \rho(u')F(3\phi, u - u')\,du', \tag{36}$$

where the limit Q is defined by the condition

$$\int_{-Q}^{Q} \rho(u)\,du = n/N = 1 - y. \tag{37}$$

The eigenvalue λ can be expressed in terms of the u_m by Eqs. (21), (25), and (33). Taking the continuum

[3] C. N. Yang and C. P. Yang, Phys. Rev. **150**, 327 (1966).

limit then gives

$$\log\frac{\lambda}{a}=\tfrac{1}{2}\int_{-Q}^{Q}du\;\rho(u)\log\left\{\frac{\cosh u-\cos 2\phi}{\cosh u-1}\times\frac{\cosh u-\cos 3\phi}{\cosh u-\cos\phi}\right\}. \quad (38)$$

When the number of up and down arrows in each row of the lattice are equal, $n=N$ and $y=0$. In this case, $Q=\infty$ and (36) can be solved by Fourier transforms, giving

$$\rho(u)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{e^{iku}\,dk}{2\cosh(k\phi)-1}. \quad (39)$$

Substituting this result into (38) and performing the integration with respect to u gives:

$$\log\frac{\lambda}{a}=P\int_{-\infty}^{\infty}\frac{dk}{k}\,\frac{(1-e^{-2k\phi})(1+e^{-k\phi})}{(e^{k\phi}-1+e^{-k\phi})(1-e^{-2k\pi})}. \quad (40)$$

Three particular cases are of special interest:

(i) $\phi=\frac{2}{3}\pi$, $b=a$, and $c=0$. The integrand in (40) is an odd function of k, so we find as expected that $\lambda=a$.

(ii) $\phi=\frac{1}{2}\pi$, $a=b=c$. This case can be regarded as the triangular-lattice equivalent of the ice model. Evaluating $\rho(u)$ explicitly from (39), substituting the resulting expression into (38) and defining a new variable of integration $t=\exp(u/3)$, we find that the integrand of (38) is an even function of t. Hence the integration can be extended over the whole of the real t axis, and on closing the contour round the upper half-plane it is found that

$$\lambda/a=\tfrac{3}{2}\sqrt{3}\simeq 2.598. \quad (41)$$

(iii) $\phi=\frac{1}{3}\pi$, $b=3a$, and $c=2a$. $w^3=-1$, so that the Eqs. (28) and (29) reduce to sets of single equations for single variables. The integration in (40) can be completed round the upper-half k plane; summing over residues then gives

$$\log\frac{\lambda}{a}=\frac{3\sqrt{3}}{\pi}\left\{\frac{1}{1^2}-\frac{1}{5^2}+\frac{1}{7^2}-\frac{1}{11^2}+\frac{1}{13^2}-\frac{1}{17^2}+\cdots\right\} \quad (42)$$

and, hence, $\lambda/a\simeq 5.03$.

7. THE CASE $c>3a$

When $c>3a$ it follows from (23) that w can be chosen to be real and greater than one. In this case $z_1,\cdots,z_n$ lie on the unit circle, so one can write

$$z_m=\exp(i\theta_m). \quad (43)$$

Define a function

$$G(w,\theta)=\frac{1}{\pi}\tan^{-1}\left\{\frac{w+1}{w-1}\tan\frac{\theta}{2}\right\} \quad (44)$$

such that $G(w,\theta)$ is a continuous function for θ for $-\pi<\theta\leqslant\pi$ and is zero when $\theta=0$. Then, on using (30) and (43), Eq. (31) becomes

$$\tfrac{1}{2}(2m-n-1)=NG(w,\theta_m)+NG(w^2,\theta_m)-\sum_{m'=1}^{n}G(w^3,\theta_m-\theta_{m'}) \quad (45)$$

for $m=1,\cdots,n$. When $y=0$ and $N\to\infty$, the θ_m's tend to a continuous distribution in the range $(-\pi,\pi)$ such that $-\pi<\theta_1<\cdots<\theta_n<\pi$ and $\theta_{n+1-m}=-\theta_m$. Letting $N\rho(\theta)$ be the density of θ_m's and proceeding as in Sec. 6, we find that

$$\rho(\theta)=\frac{1}{2\pi}\sum_{n=-\infty}^{\infty}\frac{e^{in\theta}}{w^n-1+w^{-n}}, \quad (46)$$

$$\log\frac{\lambda}{a}=2\log w+\sum_{n=1}^{\infty}\frac{1}{n}\frac{(1-w^{-2n})(1+w^{-n})}{w^n-1+w^{-n}}. \quad (47)$$

8. TRANSITION REGION $c\simeq 3a$

It is interesting to compare the forms (40) and (47) of the free energy. By deforming the contour of integration, we find that the right-hand side of (40) is an analytic function of ϕ in the upper and lower half-planes, and on the interval $(0,\pi)$ of the real axis. When ϕ lies in the upper half-plane, which from (32) implies that $|w|>1$, the integration in (40) can be completed round the upper-half k plane, giving:

$$\log\frac{\lambda}{a}=2\log w+\sum_{n=1}^{\infty}\frac{1}{n}\frac{(1-w^{-2n})(1+w^{-n})}{w^n-1+w^{-n}}+i\sqrt{3}\sum_{n=-\infty}^{\infty}\frac{6}{6n+1}\left\{1-\exp\left[\frac{2\pi^2 i}{3\phi}|6n+1|\right]\right\}^{-1}. \quad (48)$$

It is found that $\log(\lambda/a)$ can be formally expanded in powers of $(c-3a)/a$ and that the expansions are the same for c above and below $3a$. However, on comparing (47) and (48) it is apparent that $\log(\lambda/a)$ has a different analytic form in the two cases, and that the difference has an essential singularity at the transition point $\phi=0$. Thus, the system undergoes an infinite-order phase transition similar to that of the square-lattice F model.

9. SUMMARY

An ansatz solution of the triangular-lattice F model has been found when the vertex weights a, b, c satisfy the restriction (22). For such values the system undergoes an infinite-order phase transition at the point $b=7a$, $c=3a$.

When $a=b=c=1$ the model can be regarded as the triangular-lattice equivalent of the ice model, and we find that $\lambda=\frac{3}{2}\sqrt{3}\simeq 2.598$ [Eq. (41)]. A

rough estimate of this value could have been obtained by noting that for a lattice of L sites there are $3L$ bonds, but only 20 out of the possible 64 arrow configurations at a vertex are permitted. Neglecting correlations between vertices then suggests that

$$Z \simeq 2^{3L}(20/64)^L \quad \text{or} \quad \lambda \simeq 2.5. \tag{49}$$

These values can be compared with the corresponding results for the square lattice, for which the exact and approximate results are $\lambda = (\frac{4}{3})^{\frac{3}{2}} \simeq 1.540$ and $\lambda \simeq 1.5$ respectively. It is remarkable how accurate the approximations are in each case.

The author has also investigated the triangular-lattice F model by using toroidal, rather than helical, boundary conditions and, again, found that the elementary ansatz works only when the restriction (22) is satisfied. The toroidal boundary conditions have the advantage that one obtains Eq. (29), rather than (28). However, the transfer matrix is considerably more complicated.

It is interesting to note that the difficulties encountered when the restriction (22) is not satisfied are similar to those that occur in some nonplanar problems. Thus one might hope (perhaps optimistically) that a general solution of the triangular-lattice F model, if it could be obtained, would shed some light on these also.

10. ACKNOWLEDGMENT

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

Covariant Electromagnetic Potentials and Fields in Friedmann Universes*

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(Received 15 January 1969)

Electromagnetic potentials and fields are found for arbitrary four-current densities in Friedmann universes. A choice of gauge is made so that the potentials are similar to the flat-space potentials. A formalism is developed which allows the construction of potentials and fields which are covariant with respect to spatial transformations. It is shown explicitly how these potentials are related to the flat-space potentials through conformal and gauge transformations. Some features of the solutions in the finite models are discussed with reference to problems of interpretation raised recently by Katz.

1. INTRODUCTION

The Friedmann universes[1] are the most general simply connected cosmological models which satisfy the requirements of homogeneity and isotropy and which satisfy the Einstein field equations with matter taken to be a smoothed-out dust. Since observations seem to be consistent with these assumptions on the large scale,[2] the Friedmann models are usually considered to be the most accurate representation of the large-scale structure of the universe one has at present. Most of the observations which are relevant to cosmology are of electromagnetic origin. One would, therefore, desire a complete description of electromagnetism in the Friedmann universes.

Much simplification arises in the study of electromagnetism in the Friedmann models from the facts that the electromagnetic field equations are conformally invariant and that the Friedmann models are conformally related both to the static homogeneous models and to flat space.[3] One result of this is that electromagnetic signals in Friedmann universes are propagated only on the light cone, without scattering off of the Riemann tensor, or radiation tail, as in the case in a general curved space.[4]

A formal solution for the electromagnetic potentials A_μ in any conformally flat space–time has been given by Hobbs.[5] He showed that a choice of gauge could be made so that the Green's function for the potential propagates along the light cone, but did not try to find explicit expressions for the potentials for the case

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of the Friedmann models. Katz[6] has derived explicit expressions for the electromagnetic field $F_{\mu\nu}$ in the Friedmann models. In that paper, Maxwell's equations were solved first in static homogeneous models and then a conformal transformation was made to the Friedmann models. These fields, however, were valid only in a particular pseudo-rectangular coordinate system.

In this paper we derive the electromagnetic potentials and fields for the Friedmann models in a form which is covariant with respect to coordinate transformations in 3-space. This allows a considerable simplification in the expression for the potentials and fields and also makes apparent the physical interpretation of the various terms in the expressions. In Sec. 2 we state the problem to be solved and the method of solution. In Sec. 3 we derive expressions for second and higher covariant derivatives of the invariant distance which are then used in Sec. 4 to derive expressions for the potentials and fields. In Sec. 5 we show explicitly how our potentials for a point charge can be obtained from the Liénard–Wiechert potentials of flat space by a change of coordinates and change of gauge. In Sec. 6 we discuss the nature of the solution obtained, with particular reference to points raised by Katz about the solutions for the closed models.[6]

2. TRIAL POTENTIALS

The metric for the Friedmann universes can be written in the form[1,7]

$$ds^2 = g_{\mu\nu}\,dx^\mu\,dx^\nu = dt^2 - a^2(t)[d\rho^2 + f^2(\rho)\,d\Omega^2], \tag{2.1}$$

where

$$\begin{aligned} f(\rho) &= \sin\rho, \quad \text{closed 3-space } (k=+1),\\ &= \quad \rho, \quad \text{flat} \quad \text{3-space } (k=0),\\ &= \sinh\rho, \quad \text{open} \quad \text{3-space } (k=-1),\\ d\Omega^2 &= d\theta^2 + \sin^2\theta\,d\varphi^2, \end{aligned}$$

and $a(t)$ is the expansion factor which is determined by solving the field equations with matter present.[1] By a change of variables, $dt = a\,d\tau$, the metric takes the form

$$ds^2 = a^2(\tau)[d\tau^2 - (d\rho^2 + f^2(\rho)\,d\Omega^2)] \equiv a^2(\tau)\,d\tilde{s}^2, \tag{2.2}$$

which shows that the metric for the Friedmann models is conformally related to the metric for the static homogeneous models through the factor $a^2(\tau)$. Since the equations for the electromagnetic potentials A_μ,

$$A_{\mu;\lambda}{}^{;\lambda} - A_{\lambda;\mu}{}^{;\lambda} = 4\pi J_\mu, \tag{2.3}$$

are invariant under the conformal transformations

$$\begin{aligned} g_{\mu\nu} &\to g'_{\mu\nu} = e^{\Psi} g_{\mu\nu},\\ g^{\mu\nu} &\to g^{\mu\nu'} = e^{-\Psi} g^{\mu\nu},\\ A_\mu &\to A'_\mu = A_\mu,\\ J_\mu &\to J'_\mu = e^{-\Psi} J_\mu, \end{aligned} \tag{2.4}$$

the electromagnetic potentials in the Friedmann models are the same as in the static homogeneous models for conformally related sources. For this reason we will first consider the electromagnetic potentials in the static homogeneous models. Of course, the potentials are not unique because of the invariance of the field equations (2.3) under the gauge transformation

$$A'_\mu = A_\mu + \varphi_{,\mu}. \tag{2.5}$$

The electromagnetic field tensor

$$F_{\mu\nu} = A_{\mu;\nu} - A_{\nu;\mu} \tag{2.6}$$

is, however, both gauge-invariant and conformally invariant.

In the static homogeneous models there is a natural set of coordinates for which $g_{00} = 1$ and $g_{0i} = 0$. Time components of vectors and tensors then behave as scalars under transformations involving only spatial coordinates. We therefore find it desirable to find expressions for the electromagnetic potentials which are covariant with respect to transformations in 3-space. The arbitrariness associated with the gauge invariance (2.5) is removed by the assumption that the time component of the potential A_0 depends only on the time component of the current density J^0 and that the spatial components of the potential A_i depend only on the spatial components of the current density J^k. This assumption is made in analogy with the structure of the solution for the potentials in flat space in the Lorentz gauge. However, it should be noted that the curved-space solutions which satisfy the above criteria may not satisfy the curved-space analog of the Lorentz gauge, i.e., $A_\mu{}^{;\mu} = 0$.

Because the Friedmann models, and thus also the static homogeneous models, are conformally flat,[3] the electromagnetic field $F_{\mu\nu}(\mathbf{x}, \tau)$ depends on the current density $J^\mu(\mathbf{x}', \tau')$ only at the retarded time τ' given by

$$\tau' = \tau - \Psi(\mathbf{x}, \mathbf{x}'), \tag{2.7}$$

where $\Psi(\mathbf{x}, \mathbf{x}')$ is the biscalar distance between the

[6] A. Katz, J. Math. Phys. **9**, 1964 (1968).

[7] Greek indices take values from 0 to 3; Latin indices are restricted to spatial components 1 to 3. The signature of our metric is -2. We adopt a system of units in which $c = 1$. Covariant differentiation will be denoted by a semicolon (;), ordinary differentiation by a comma (,).

points $\mathbf{x}$ and $\mathbf{x}'$, measured along a geodesic[8] in the 3-space which joins the points $\mathbf{x}$ and $\mathbf{x}'$. We assume that the potentials also have this property of being sharply propagated along the light cone. The general form of A_0 which incorporates this dependence is then

$$A_0(\mathbf{x}, \tau) = \int F(\Psi) J^0(\mathbf{x}', \tau') \delta(\tau' - \tau + \Psi)\, d^4V', \quad (2.8)$$

where $d^4V' = (-g)^{\frac{1}{2}}\, d^4x'$ and $F(\Psi)$ is a function of the invariant distance between $\mathbf{x}$ and $\mathbf{x}'$ which will be determined by substitution into the field of equations (2.3).

The trial solution for the spatial components of the potential, A_i, requires the use of some bivector $C_{ij'}(\mathbf{x}, \mathbf{x}')$ to relate the current density at $\mathbf{x}'$ to the potential at $\mathbf{x}$. Geometrical bivectors[4] can be formed from the parallel propagator[9] $g_{ij'}$, and first and higher derivatives of the invariant distance, e.g., $\Psi_{,i}\Psi_{,j'}$, etc. However, we will show that, in the static homogeneous models, second and higher derivatives of Ψ can be reduced to first derivatives of Ψ, the parallel propagator, and known scalar functions of the invariant distance Ψ. It therefore suffices to consider the trial solution

$$A_k(\mathbf{x}, \tau') = -\int [g_{km'} G(\Psi) + \Psi_{;k}\Psi_{;m'} H(\Psi)] J^{m'}(\mathbf{x}', \tau') \times \delta(\tau' - \tau + \Psi)\, d^4V'. \quad (2.9)$$

The functions $F(\Psi)$, $G(\Psi)$, and $H(\Psi)$ are determined by substituting (2.8) and (2.9) into the field equations (2.3). However, in order to reduce the resulting expressions, we must know how to express derivatives of $g_{ij'}$ and higher than first derivatives of Ψ in terms of simpler quantities. Synge[9] has given such expressions for the general case of an expansion in powers of the Riemann tensor which one finds useful for approximation methods. For the static homogeneous models, we can derive exact expressions for these derivatives, so that we do not have to assume that the Riemann tensor is small. This derivation is done in the next section.

3. GEOMETRICAL RELATIONS

The world function[9] $\Omega(\mathbf{x}, \mathbf{x}')$ for the 3-space is related to the invariant distance $\Psi(\mathbf{x}, \mathbf{x}')$ by

$$\Omega = \tfrac{1}{2}\Psi^2. \quad (3.1)$$

Since

$$\Omega_{;k}\Omega^{;k} = \Omega_{;k'}\Omega^{;k'} = 2\Omega, \quad (3.2)$$

the derivatives of Ψ satisfy

$$\Psi_{;k}\Psi^{;k} = \Psi_{;k'}\Psi^{;k'} = 1. \quad (3.3)$$

Therefore, $\Psi_{;k}$ is a unit vector at $\mathbf{x}$ directed tangent to the geodesic from $\mathbf{x}'$ to $\mathbf{x}$ and $\Psi_{;k'}$ is a unit vector at $\mathbf{x}'$ directed tangent to the geodesic from $\mathbf{x}$ to $\mathbf{x}'$. The bivector parallel propagator[9] $g_{ij'}(\mathbf{x}, \mathbf{x}')$ relates components of a vector A_i at a point $\mathbf{x}$ to the components of that same vector parallel-transported along the geodesic joining the two points $\mathbf{x}$ and $\mathbf{x}'$:

$$A_i = g_{ij'}A^{j'}, \quad A_{j'} = g_{j'i}A^i. \quad (3.4)$$

Derivatives of Ω and Ψ with respect to $\mathbf{x}$ are related to those with respect to $\mathbf{x}'$ by the parallel propagator

$$\Omega_{;k} = -g_{km'}\Omega^{;m'}, \qquad \Psi_{;k} = -g_{km'}\Psi^{;m'}, \quad (3.5)$$

from which it follows that, if $f(\Psi)$ is any function of Ψ,

$$f_{;k} = -g_{km'}f^{;m'}. \quad (3.6)$$

The relationship between the derivatives of Ω and Ψ and the parallel propagator can be derived from the relations written down by Synge,[9] applied to our particular case of a 3-space of constant curvature. We consider a two-dimensional family of geodesics radiating from a fixed point P (coordinates x^i) with affine parameter u along the geodesics and parameter v which varies continuously from geodesic to geodesic. This determines a 2-space $x^i \equiv x^i(u, v)$ in which we have

$$U^i = \frac{\partial x^i}{\partial u}, \quad V^i = \frac{\partial x^i}{\partial v}, \quad (3.7)$$

where U^i is the unit tangent vector along the geodesics and V^i is proportional to the deviation vector between adjacent geodesics. From the relations (3.7) we have

$$\frac{\delta U^i}{\delta v} = \frac{\delta V^i}{\delta u}, \quad \frac{\delta U^i}{\delta u} = 0, \quad (3.8)$$

where $\delta/\delta v$ (or $\delta/\delta u$) implies absolute differentiation along the curve $u = \text{const}$ (or $v = \text{const}$).

If we consider a point $\bar{P}$ (coordinates $\bar{x}^i$) lying on a curve $C(v)$ with constant parameter $\bar{u}$, then we have from the relations of Synge[9] that

$$\Omega_{;i} = -\Delta u\, U_i, \quad \Omega_{;\bar{i}} = \Delta u\, U_{\bar{i}}, \quad (3.9)$$

and

$$\Omega = \tfrac{1}{2}\Psi^2 = \tfrac{1}{2}(\Delta u)^2, \quad (3.10)$$

where $\Delta u = \bar{u} - u$. The relations involving derivatives of Ω are obtained by Synge by varying the end point

[8] In the $k = +1$, closed models, there is more than one geodesic joining the two points and, therefore, more than one Ψ. We assume that all possible Ψ's contribute. This point is discussed further in Sec. 6.

[9] J. L. Synge, *Relativity: The General Theory* (North-Holland Publ. Co., Amsterdam, 1960), Chap. II.

$\bar{P}$ along the curve $C(v)$. This results in the equalities

$$\Omega_{;k;\bar{m}}V^{\bar{m}} = -\Delta u\frac{\delta U_k}{\delta v} = -\Delta u\frac{\delta V_k}{\delta u}$$
$$= -g_{k\bar{m}}V^{\bar{m}} - \int_u^{\bar{u}}[(\bar{u}-u')K^{j'i'}g_{kj'}V_{i'}]\,du', \tag{3.11}$$

$$\Omega_{;\bar{k};\bar{m}}V^{\bar{m}} = \Delta u\frac{\delta U_{\bar{k}}}{\delta v} = \Delta u\frac{\delta V_{\bar{k}}}{\delta u}$$
$$= V_{\bar{k}} - \int_u^{\bar{u}}[(u'-u)K^{j'i'}g_{\bar{k}j'}V_{i'}]\,du', \tag{3.12}$$

where the affine parameter is u at P, $\bar{u}$ at $\bar{P}$, and u' at intermediate points P' along the geodesic between P and $\bar{P}$. K_{ij} is given by

$$K_{ij} = R_{ikjm}U^kU^m \tag{3.13}$$

and V^i satisfies the equation of geodesic deviation

$$\frac{\delta^2V^i}{\delta u^2} + K^i_mV^m = 0. \tag{3.14}$$

For the case of static homogeneous universes, the spatial Riemann tensor is

$$R_{ikjm} = \lambda[g_{ij}g_{km} - g_{im}g_{jk}], \tag{3.15}$$

with $\lambda = k/r_0^2$, where $k = +1, 0, -1$ corresponds to a closed, flat, or open model and r_0 is the radius of curvature of the 3-space. Since the static homogeneous models will be related to the Friedmann models by a conformal transformation, we may, without loss of generality, choose $r_0 = 1$. Also we will derive in detail the results only for the closed model $k = +1$, the other cases being found in a similar manner. Since $U^iU_i = 1$, we have, from (3.15) and (3.13),

$$K_{ij} = g_{ij} - U_iU_j\,, \tag{3.16}$$

so that the equation of geodesic deviation (3.14) becomes

$$\frac{\delta^2V^i}{\delta u^2} + [V^i - U^iV_jU^j] = 0. \tag{3.17}$$

We now break up V^i into parts parallel and perpendicular to the geodesic

$$V^i = (U^iV^jU_j) + (V^i - U^iV_jU^j)$$
$$\equiv V^i_{\parallel} + V^i_{\perp} \tag{3.18}$$

and since $\delta(V^jU_j)/\delta u = 0$, we then have that

$$\frac{\delta^2V^i_{\parallel}}{\delta u^2} = 0,$$
$$\frac{\delta^2V^i_{\perp}}{\delta u^2} + V^i_{\perp} = 0. \tag{3.19}$$

The solutions to these equations for $V^{i'}$ at an intermediate point with parameter u' are then

$$V^{i'}_{\parallel} = g^{i'}_{\bar{m}}V^{\bar{m}}_{\parallel}\left[\frac{u'-u}{\bar{u}-u}\right],$$
$$V^{i'}_{\perp} = g^{i'}_{\bar{m}}V^{\bar{m}}_{\perp}\left[\frac{\sin(u'-u)}{\sin(\bar{u}-u)}\right], \tag{3.20}$$

where the two constants of integration are chosen so that $V^{i'} \to 0$ when $u' \to u$ and $V^{i'} \to V^{\bar{i}}$ when $u' \to \bar{u}$. The parallel propagator is, of course, a constant under absolute differentiation along the geodesic.

When the expression for K_{ij}, Eq. (3.16), is substituted into (3.11) and (3.12), one finds that the only contribution to the integrals in those two expressions come from $V_{\perp j'}$. The expression for $V_{\perp j'}$ from (3.20) allows us to explicitly perform the integrations in (3.11) and (3.12). Making use of the defining relations for $V_{\perp j'}$, Eq. (3.18), then leads to the two expressions

$$\Omega_{;k;\bar{m}}V^{\bar{m}} = -U_kU_{\bar{m}}V^{\bar{m}} - \frac{(\bar{u}-u)}{\sin(\bar{u}-u)}$$
$$\times [g_{k\bar{m}}V^{\bar{m}} - U_kU_{\bar{m}}V^{\bar{m}}], \tag{3.21}$$

$$\Omega_{;\bar{k};\bar{m}}V^{\bar{m}} = U_{\bar{k}}U_{\bar{m}}V^{\bar{m}} + (\bar{u}-u)\cot(\bar{u}-u)$$
$$\times [V_{\bar{k}} - U_{\bar{k}}U_{\bar{m}}V^{\bar{m}}]. \tag{3.22}$$

Since the $V^{\bar{m}}$ are arbitrary, the coefficients of $V^{\bar{m}}$ must be equal on each side of each expression. Using Eqs. (3.9) and (3.10), and rewriting for the case of a general $\Psi(\mathbf{x}, \mathbf{x}')$, we find that, including the $k = 0$ and $k = -1$ cases, which follow similarly:

$$\Psi_{;k;m'} = -y(\Psi)[g_{km'} + \Psi_{;k}\Psi_{;m'}],$$
$$\Psi_{;k;m} = +z(\Psi)[g_{km} - \Psi_{;k}\Psi_{;m}], \tag{3.23}$$

where

$$y(\Psi) = \csc\Psi, \quad k = +1,$$
$$= 1/\Psi, \quad k = 0,$$
$$= \operatorname{csch}\Psi, \quad k = -1,$$
$$z(\Psi) = \cot\Psi, \quad k = +1,$$
$$= 1/\Psi, \quad k = 0,$$
$$= \coth\Psi, \quad k = -1.$$

The only other relation we need is an expression for the derivatives of the parallel propagator $g_{km'}$. Again we make use of the equation given by Synge[9] which considers the change in the parallel propagator as the end point $\bar{P}$ is moved along the curve $C(v)$:

$$g_{km;\bar{n}}V^{\bar{n}} = -\int_u^{\bar{u}}[g_{ki'}g_{mj'}R^{i'j'a'b'}V_{a'}U_{b'}]\,du'. \tag{3.24}$$

When the expression for the Riemann tensor (3.15) is substituted into (3.24), we again find that only $V_{\perp a'}$

contributes to the integral. Using the derived expression for $V_{\perp a'}$, Eq. (3.20), we can evaluate the integral in (3.24) to give

$$g_{km;\bar{n}}V^{\bar{n}} = -\tan(\tfrac{1}{2}\Psi)[V_k U_m - U_k g_{m\bar{n}}V^{\bar{n}}]. \quad (3.25)$$

Since this must hold for arbitrary $V^{\bar{n}}$, we have for the general case, including the results of the similar derivations for $k = 0$ and $k = -1$,

$$g_{k'm;n'} = w(\Psi)[g_{k'n'}\Psi_{;m} + g_{mn'}\Psi_{;k'}], \quad (3.26)$$

where

$$\begin{aligned} w(\Psi) &= \tan\tfrac{1}{2}\Psi, & k &= +1, \\ &= 0, & k &= 0, \\ &= -\tanh\tfrac{1}{2}\Psi, & k &= -1. \end{aligned}$$

Equations (3.23) and (3.26) allow us to reduce any expression involving higher than first derivatives of Ψ and any derivatives of $g_{ij'}$ to expressions involving only Ψ, $g_{ij'}$, and first derivatives of Ψ. This is required for our derivation in the next section.

4. DETERMINATION OF THE POTENTIALS AND FIELDS

The trial potentials (2.8) and (2.9) are now substituted in the field equations (2.3) to find what restrictions are placed on the functions $F(\Psi)$, $G(\Psi)$, and $H(\Psi)$. Because of current conservation

$$J_{;\mu}{}^{\mu} = \frac{\partial J^0}{\partial \tau} + J^k_{;k} = 0, \quad (4.1)$$

time derivatives of the charge density J^0 can be expressed as the divergence of the current density J^k. Whenever we have a $J^{0'}$ together with a derivative of the δ function in (2.8) and (2.9), we can integrate by parts with respect to τ' and use (4.1) to express $\partial J^{0'}/\partial\tau'$ as the divergence of the current density, $J_{;k'}{}^{k'}$. The derivative with respect to the k' can likewise be integrated by parts, leaving $J^{k'}$ without any derivatives. We will reduce terms in this way whenever possible so that the possible forms of the terms in our expressions are independent of each other for arbitrary J_μ. We further reduce expressions through the use of relations (3.23) and (3.26) so that only Ψ, $g_{ik'}$, and first derivatives of Ψ appear in the final expressions. After these reductions are made, we are left with a series of differential equations for the unknown functions F, G, and H, which we then solve using appropriate boundary conditions.

The function $F(\Psi)$ in (2.8) may be determined by considering the particular case where $J^k = 0$ and J^0 is, therefore, time-independent. In this case the condition on $F(\Psi)$ from (2.8) and (2.3) is

$$4\pi J^0 = -A_{0;k}{}^{;k} = -\int J^{0'}F^{;k}_{;k}\delta(\tau' - \tau + \Psi)\, d^4V', \quad (4.2)$$

where terms resulting from differentiation of the δ function vanish since $J^{0'}$ is time-independent. The condition which F must satisfy is therefore

$$F^{;k}_{;k} = -4\pi\delta^3(\mathbf{x} - \mathbf{x}')/(-g')^{\frac{1}{2}}, \quad (4.3)$$

where, from (3.3) and (3.23),

$$F^{;k}_{;k} = F'' + 2F'\cot\Psi. \quad (4.4)$$

The general solution of (4.3) and (4.4) is

$$F = \cot\Psi + C, \quad (4.5)$$

where C is a constant of integration.

Surprisingly, the functions G and H in (2.9) can also be determined from the equation for J^0 if we consider the case of arbitrary J^μ. This means that the functions F, G, and H are over-determined since this procedure does not yet utilize any information contained in the field equations with J^k as the source. After finding G and H, we must therefore show that they are consistent with these latter equations as well. When (2.8) and (2.9), with $F = \cot\Psi + C$, are substituted in Eq. (2.3) with $\mu = 0$, we find from relations (3.23) and (3.26) that G and H must satisfy the equation

$$\begin{aligned} \int\{J^{0'}[(\cot\Psi + C)\delta'' + (2C\cot\Psi - 2)\delta'] \\ + \Psi_{;k'}J^{k'}[(G - H)\delta'' + (G' - H' - 2G\tan\tfrac{1}{2}\Psi \\ - 2H\cot\Psi)\delta']\}\, d^4V' = 0, \end{aligned} \quad (4.6)$$

where $\delta \equiv \delta(\tau' - \tau + \Psi)$ and a prime on G, H, and δ indicates differentiation with respect to the argument. The terms in $J^{0'}$ can be reduced to terms in $J^{k'}$ by first integrating by parts with respect to τ', using (4.1), and then integrating by parts with respect to $x^{k'}$. This yields the condition

$$\begin{aligned} \int\Psi_{;k'}J^{k'}[(G - H - \cot\Psi - C)\delta'' \\ + (G' - H' - 2G\tan\tfrac{1}{2}\Psi - 2H\cot\Psi \\ + 2 - \csc^2\Psi - 2C\cot\Psi)\delta' \\ + (2C\csc^2\Psi)\delta]\, d^4V' = 0. \end{aligned} \quad (4.7)$$

Because (4.7) must hold for arbitrary $J^{k'}$, the coefficients of δ'', δ', and δ must vanish separately since these indicate different order time derivatives of $J^{k'}$. From the coefficient of δ we find that $C = 0$. Requiring the coefficient of δ'' vanishes gives $G = H + \cot\Psi$ which, when substituted into the coefficient of δ', gives the unique solution

$$H = \tan\tfrac{1}{2}\Psi; \quad G = \csc\Psi. \quad (4.8)$$

Thus far we have found the potentials by using the trial potentials (2.8) and (2.9) in the field equations (2.3) with $\mu = 0$. We have to verify that our potentials are solutions of these equations with $\mu = k$ as well. This procedure is carried out in a straightforward manner. The result is that our potentials are solutions of the full set of Eqs. (2.3). Including the similar results for $k = 0$ and $k = -1$, we now state our solution to be the potentials (2.8) and (2.9) with the functions F, G, and H given by

$$\begin{aligned} F(\Psi) &= \cot\Psi, && k = +1, \\ &= 1/\Psi, && k = 0, \\ &= \coth\Psi, && k = -1, \\ G(\Psi) &= \csc\Psi, && k = +1, \\ &= 1/\Psi, && k = 0, \\ &= \operatorname{csch}\Psi, && k = -1, \\ H(\Psi) &= \tan\tfrac{1}{2}\Psi, && k = +1, \\ &= 0, && k = 0, \\ &= -\tanh\tfrac{1}{2}\Psi, && k = -1. \end{aligned} \tag{4.9}$$

By explicit calculation we find that

$$A_\mu{}^{;\mu} = 2\int \Psi_{;k'}J^{k'}\delta(\tau' - \tau + \Psi)\, d^4V', \tag{4.10}$$

for the cases $k = +1$ and $k = -1$, and $A_\mu{}^{;\mu} = 0$ for $k = 0$.

The electromagnetic field $F_{\mu\nu}$, which is the physically meaningful quantity, is found from the potentials using (2.6). Again whenever a $J^{0'}$ appears together with a δ', we reduce this to a $J^{k'}$ term as before. The electromagnetic field thus derived for the three cases is

$$\begin{aligned} F_{0k} = \int \{&G(\Psi)[g_{km'} + \Psi_{;k}\Psi_{;m'}]J^{m'}[F(\Psi)\delta - \delta'] \\ &+ G^2(\Psi)[\Psi_{;k}\Psi_{;m'}J^{m'} - \Psi_{;k}J^{0'}]\delta\}\, d^4V', \end{aligned} \tag{4.11}$$

$$\begin{aligned} F_{km} = \int \{&G(\Psi)[g_{kn'}\Psi_{;m} - g_{mn'}\Psi_{;k}]J^{n'} \\ &\times [F(\Psi)\delta - \delta']\}\, d^4V', \end{aligned} \tag{4.12}$$

where $F(\Psi)$ and $G(\Psi)$ are given in (4.9) and $\delta = \delta(\tau' - \tau + \Psi)$.

The electromagnetic potentials and fields thus given by (2.8), (2.9), (4.11), (4.12), together with (4.9), are those appropriate for a static, homogeneous cosmological model having a metric given by $d\bar{s}$ in Eq. (2.2). To express the solution in terms of the metric ds of Eq. (2.2) it is necessary to conformally transform the quantities appearing in the solution according to (2.4). Both A_μ and $F_{\mu\nu}$ are invariant, but $J^{\mu'} \to a^4(t')J^{\mu'}$ under this transformation. Usually the Friedmann models are given as the metric (2.1) in which comoving coordinates are chosen for the matter in the universe. (2.1) is obtained from (2.2) by a coordinate transformation $d\tau = dt/a(t)$, so that any time components of vectors in our expressions undergo a transformation as well. Also we can write $d^4V' = d\tau'\, d^3V' = a^{-1}\, dt'\, d^3V' = a^{-4}(-g')^{\frac{1}{2}}\, d^4x'$. Therefore we can write our result for the electromagnetic potentials and fields in the Friedmann models in the metric of (2.1) as

$$A_0(\mathbf{x}, t) = \frac{1}{a(t)}\int \frac{F(\Psi)}{a(t')}J^0(\mathbf{x}', t')\delta(s)(-g')^{\frac{1}{2}}\, d^4x', \tag{4.13}$$

$$\begin{aligned} A_k(\mathbf{x}, t) = -\frac{1}{a(t)}\int &\frac{[d_{km'}G(\Psi) + n_k n_{m'}H(\Psi)]}{a(t')} \\ &\times J^{m'}(\mathbf{x}', t')\delta(s)(-g')^{\frac{1}{2}}\, d^4x', \end{aligned} \tag{4.14}$$

$$\begin{aligned} F_{0k}(\mathbf{x}, t) = \frac{1}{a^2(t)}\int \Big\{&\frac{G(\Psi)}{a(t')}[d_{km'} + n_k n_{m'}] \\ &\times J^{m'}(\mathbf{x}', t')[F(\Psi)\delta(s) - \delta'(s)] \\ &+ \frac{G^2(\Psi)}{a(t')}[n_k n_{m'}J^{m'}(\mathbf{x}', t') \\ &- n_k J^{0'}(\mathbf{x}', t')]\delta(s)\Big\}(-g')^{\frac{1}{2}}\, d^4x', \end{aligned} \tag{4.15}$$

$$\begin{aligned} F_{km}(\mathbf{x}, t) = \frac{1}{a^2(t)}\int \Big\{&\frac{G(\Psi)}{a(t')}[d_{kl'}n_m - d_{ml'}n_k]J^{l'}(\mathbf{x}', t') \\ &\times [F(\Psi)\delta(s) - \delta'(s)]\Big\}(-g')^{\frac{1}{2}}\, d^4x', \end{aligned} \tag{4.16}$$

where

$$s = \int_t^{t'} \frac{dt''}{a(t'')} + \Psi(\mathbf{x}, \mathbf{x}'), \tag{4.17}$$

$$n_k = a(t)\Psi_{;k}, \quad n_{k'} = a(t')\Psi_{;k'}, \tag{4.18}$$

$$d_{km'} = a(t)a(t')g_{km'}, \tag{4.19}$$

and F, G, and H are given by (4.9). Quantities with spatial indices now have the tensoral properties associated with the metric (2.1) so that, e.g.,

$$n_k n^k = n_k n_l g^{kl} = -(1/a^2)(a\Psi_{;k})(a\Psi_{;l})g^{kl}_{(3)} = -1,$$

where $g^{kl}_{(3)}$ is the positive-signature metric of the space of constant curvature.

A simple physical interpretation can be given to the quantities in (4.13)–(4.16). $\Psi(\mathbf{x}, \mathbf{x}')$ can be expressed as $L(\mathbf{x}, \mathbf{x}', t)/a(t)$, where L is physical distance between the points $\mathbf{x}$ and $\mathbf{x}'$ at some time t. n_k is a unit vector at $\mathbf{x}$ directed along the geodesic in the 3-space of constant t from $\mathbf{x}'$ to $\mathbf{x}$, with a similar interpretation for $n_{k'}$. $d_{km'}$ parallel propagates the direction of the current density $J^{m'}$ from $\mathbf{x}'$ to $\mathbf{x}$ along the geodesic without

changing any magnitudes. The $\delta(s)$ indicates simply that electromagnetic influences propagate only along null geodesics.

The potentials and fields of a charge q can be found using the expression for the 4-current density

$$J^\mu(x) = q\int \frac{dz^\mu}{ds}\frac{\delta^4(x - z(s))}{(-g)^{\frac{1}{2}}}\,ds, \tag{4.20}$$

where $x^\mu = z^\mu(s)$ is the parametric equation of the path. Substituting (4.20) into (4.13) and (4.14) gives the potentials (analogous to the Liénard–Wiechert potentials):

$$A_0(\mathbf{x}, t) = \frac{qF(\Psi')}{a(t)\sigma}, \tag{4.21}$$

$$A_k(\mathbf{x}, t) = -\frac{q[G(\Psi')\,d_{km'} + H(\Psi')n_k n_{m'}]v^{m'}(t')}{a(t)\sigma}, \tag{4.22}$$

where the path has been taken to be $\mathbf{z}(t')$, t' being the retarded time obtained from setting $s = 0$ in (4.17). Ψ' is shorthand for $\Psi(\mathbf{x}, \mathbf{z}(t'))$. $\sigma \equiv 1 + n_{k'}v^{k'}(t')$ and $v^{k'} = dz^k(t')/dt'$. The fields can be found in a similar manner.

5. TRANSFORMATION FROM FLAT SPACE

Since the Friedmann models are conformally flat, it should be possible to derive the potentials and fields from the flat-space potentials and fields using the conformal transformations (2.4), coordinate transformations, and possibly gauge transformations. Since we showed in Sec. 4 how the potentials in the Friedmann models can be obtained from those in the static homogeneous models, it will suffice to show that the potentials (2.8) and (2.9) in the static homogeneous models can be obtained from the usual flat-space Liénard–Wiechert potentials.[10] To simplify the procedure, we assume that we have the $k = +1$ model, whose metric is

$$ds^2 = d\tau^2 - d\rho^2 - \sin^2\rho\,d\Omega^2. \tag{5.1}$$

We consider the case of a point charge which is at the origin $\rho' = 0$ at the retarded time $\tau' = 0$, so that the potential we write will be valid at coordinate ρ only at the time $\tau = \rho$. We assume that the velocity of the charge is in the $\theta = 0$ direction. The appropriate potentials are then just (4.21) and (4.22) with $a = 1$, $\Psi' = \rho$, since ρ is the physical distance from the origin measured radially outward. The only quantities which we need to evaluate explicitly in (4.22) are the components of the parallel propagator $g_{km'}$. Consider the change in a vector as it is parallel propagated radially, which is along a geodesic in 3-space. Then

$$dv^i = -\begin{Bmatrix} i \\ j\ k \end{Bmatrix}v^j\,dx^k = -\begin{Bmatrix} i \\ j\ l \end{Bmatrix}v^j\,d\rho. \tag{5.2}$$

From (5.2) and the metric (5.1), we see that the radial component of the velocity vector is unchanged under parallel transport. Thus $g_{11'} = 1$. But since the magnitude of v is unchanged, this implies also that v_2v^2 is unchanged under the transport (5.2), which may also be explicitly verified from (5.2). Therefore, the potentials with the metric (5.1) are explicitly given as

$$\begin{aligned} A_0 &= \frac{q\cot\rho}{1 - v\cos\theta}, \\ A_1 &= -\frac{qv\cot\rho\cos\theta}{1 - v\cos\theta}, \\ A_2 &= \frac{qv\sin\theta}{1 - v\cos\theta}, \end{aligned} \tag{5.3}$$

which are valid at coordinate ρ at the time $\tau = \rho$.

The metric for flat space may be taken to be

$$ds^2 = dt^2 - dr^2 - r^2\,d\Omega^2, \tag{5.4}$$

in which the flat-space potentials in the Lorentz gauge for a charge at the origin $r' = 0$ at time $t' = 0$ are

$$\begin{aligned} A_0 &= \frac{q}{r(1 - v\cos\theta)}, \\ A_1 &= -\frac{qv\cos\theta}{r(1 - v\cos\theta)}, \\ A_2 &= \frac{qv\sin\theta}{(1 - v\cos\theta)}, \end{aligned} \tag{5.5}$$

where again the expressions are valid only at the time $t = r$. The succession of coordinate transformations[3]

$$\begin{aligned} t + r &= \tan\xi, \\ t - r &= \tan\eta, \\ \xi - \eta &= \rho, \\ \xi + \eta &= \tau \end{aligned} \tag{5.6}$$

transforms (5.4) into the form

$$ds^2 = \tfrac{1}{4}\sec^2\tfrac{1}{2}(\tau + \rho)\sec^2\tfrac{1}{2}(\tau - \rho) \times [d\tau^2 - d\rho^2 - \sin^2\rho\,d\Omega^2], \tag{5.7}$$

which is just a conformal transformation of the static homogeneous metric[11] (5.1). Since A_μ is unchanged under a conformal transformation, the potentials (5.5) when transformed by the coordinate transformations

[10] Reference 1, Chapter 8.

[11] The transformation is not globally valid since the two spaces have different topological properties. This presents no problem for our treatment here since we can easily extend the transformed space–time to that of the static homogeneous one.

(5.6) should agree with the curved space–time potentials (5.3) up to a gauge transformation. Note that the point $t = r = 0$ coincides with the point $\tau = \rho = 0$, the position of the charge. Also the condition that $t = r$ in (5.5) is the same condition that $\tau = \rho$ in (5.3) as required by the fact that both potentials have a contribution from the source only at the retarded time.

If we denote by a bar quantities referred to the coordinate system defined by (5.7), then the relation between the barred and unbarred potentials is

$$\bar{A}_0 = \frac{1 + \cos\tau\cos\rho}{(\cos\tau + \cos\rho)^2} A_0 + \frac{\sin\tau\sin\rho}{(\cos\tau + \cos\rho)^2} A_1,$$
$$\bar{A}_1 = \frac{1 + \cos\tau\cos\rho}{(\cos\tau + \cos\rho)^2} A_1 + \frac{\sin\tau\sin\rho}{(\cos\tau + \cos\rho)^2} A_0,$$
$$\bar{A}_2 = A_2. \tag{5.8}$$

When we substitute the potentials (5.5) into (5.8), use the relation $r = \sin\rho/(\cos\tau + \cos\rho)$, and set $\tau = \rho$, we find that the barred potentials can be written as

$$\bar{A}_0 = \frac{q\cot\rho}{1 - v\cos\theta} + \frac{q}{2}\tan\rho,$$
$$\bar{A}_1 = -\frac{qv\cot\rho\cos\theta}{1 - v\cos\theta} + \frac{q}{2}\tan\rho, \tag{5.9}$$
$$\bar{A}_2 = \frac{qv\sin\theta}{1 - v\cos\theta}.$$

These are just the potentials (5.3) in the static homogeneous model aside from the $(q/2)\tan\rho$ term. However, since this term does not depend on the velocity of the charge v, we can find a gauge function $\varphi(\rho, \tau)$ such that $\varphi_{,0}(\rho, \rho) = \varphi_{,1}(\rho, \rho) = -\frac{1}{2}q\tan\rho$. The gauge transformation

$$\varphi = \tfrac{1}{2}q\ln[\cos\rho + \cos\tau] \tag{5.10}$$

thus transform the potentials (5.9) into (5.3), the potentials we had derived for the static, homogeneous case.

6. DISCUSSION OF SOLUTIONS

In the previous sections we have derived expressions for the electromagnetic potentials and fields for the cases of static homogeneous models and for the Friedmann universes in systems of comoving coordinates. These solutions were given in a form which is covariant with respect to coordinate transformations in 3-space. The potentials and fields derived have the property of being sharply propagated on the light cone, a consequence of the fact that the geometries considered were conformally flat. Our expressions for the fields (4.11) and (4.12) reduce to those of Katz[6] when quantities are evaluated in the particular coordinate system he used. Also we have shown that our potentials are consistent with the potentials obtained from flat space, in agreement with Hobbs.[5]

An examination of the solution we have obtained raises a few points, which we will now consider. First it should be noted that the $k = 0$ case of (2.8), (2.9), (4.11), and (4.12) is just flat space–time, and therefore the potentials and fields we have derived for this case are just the usual Lorentz gauge potentials and fields of flat space, written in a form which is covariant with respect to spatial transformations. The $k = 0$ solutions for the Friedmann models (4.13)–(4.16) are, of course, related to the flat-space ones by a simple coordinate change in the time variable. In the $k = 0$ case there is no problem concerning uniqueness of the solution, aside from the choice of gauge and causality condition chosen, in our case chosen so that we have only the retarded solution.

The $k = -1$, or open 3-space, models present an apparent difficulty in the solution for the potentials (2.8) and (2.9), with functions given by (4.9). If we let the spatial distance Ψ from the source become very large, we find that the potentials do not approach zero. This arises since $F(\Psi) \to 1$ and $H(\Psi) \to 1$ as $\Psi \to \infty$. This is also reflected in the gauge condition (4.10), which is independent of the magnitude of Ψ. However, this arises purely from our choice of gauge, which we determined by the conditions imposed on the trial potentials (2.8) and (2.9). The electromagnetic fields (4.11) and (4.12), which are the physically measurable quantities, are seen to approach zero for large Ψ, since $F_{\mu\nu} \sim 0(\exp - \Psi)$ as $\Psi \to \infty$. As with the $k = 0$ solution, uniqueness of the solution presents no problem.

The $k = +1$, or closed model solutions present the most difficulty in interpretation. This arises from the fact that in the closed, static models, there is more than one geodesic in the 3-space between any two points. In the trial solutions (2.8) and (2.9), we stated that τ, the potential at $\mathbf{x}$, should depend on the source at $\mathbf{x}'$ only at the retarded time τ', where $\tau' = \tau - \Psi(\mathbf{x}, \mathbf{x}')$. $\Psi(\mathbf{x}, \mathbf{x}')$ was the distance between the two points $\mathbf{x}$ and $\mathbf{x}'$ measured along a geodesic in the 3-space joining the points. If the two points are not opposite each other on the spherical model of radius R, then there are two Ψ's for these points which are less than $2\pi R$ and an infinite number of possible Ψ's (and therefore an infinite number of retarded times) obtained from these two by the addition of $2\pi nR$, where n is an integer. In the case of opposite points, there are an infinite number of geodesics between the two points, but each with the same smallest distance

πR, to which we may again add $2\pi nR$ for the distances along geodesics which wrap around more than once. We have a number of possible choices to make as to which Ψ's, and therefore which retarded times, one allows in the solutions. Simplicity would indicate that we accept either all of them, with a contribution to the potential from the source at each retarded time, or we accept only the shortest distance, as Katz assumed, with a single contribution to the potential from the source at the single retarded time.

Accepting all Ψ's leads to difficulties immediately in discussing the potentials and fields of a single charge. This is most easily seen in the case of a stationary charge. At some point on the model we then find a finite contribution to the field at a particular time due to the source at each retarded time, which produces an indefinite field when summed over all retarded times. Of course, what is inconsistent here is that there must be zero net charge in a closed model,[12] and one must include the contribution from some charge with the opposite sign as well. Choosing only the shortest Ψ leads to the vanishing of the effect of the source on the potential and field for $\tau - \tau' > \pi$. As Katz showed, this implies the existence of an equal and opposite charge at the opposite point, undergoing a motion similar to that of the original charge, and surrounded by a field which would be interpreted as an advanced, rather than retarded, one. However, by judiciously superimposing solutions for pairs of charges in this case, one can reproduce solutions which contain only the retarded fields for arbitrarily moving pairs of charges at any given time, and which, in fact, can reproduce the field and potentials obtained by accepting all Ψ's as above. However, this is by no means the only solution possible.

The questions posed here may be a result of the high degree of symmetry in the closed spherical models. One can picture the field generated by a source at τ' being propagated outward in all directions and then being focused by the geometry to produce a singular field at the opposite point at the time $\tau = \tau' + \pi R$. The field could then be cut off by assuming an opposite charge was present, following Katz, or one could assume that the field would continue to propagate away from the opposite point, where now no charge is assumed to exist. The latter corresponds to accepting all Ψ's in finding the contributions to the fields. If the high degree of symmetry were not present, as would realistically be the case since matter is not in fact smoothed out, geodesics radiating outward from the source would not in general converge to a point on the opposite side of the model, and one could not assume the existence of a single charge to cut off this field. The field must then continue to propagate past the opposite side. Moreover, such models would not be conformally flat, and the electromagnetic signals would then be smeared by scattering off of the Riemann tensor and not propagated sharply along the light cone. Therefore, we conclude that the physically acceptable solution for the closed static homogeneous model is that for which we admit contributions from the source at all retarded times.

Considering the case of the closed Friedmann models raises the same points, except that the discussion about geodesics which wrap around the model more than once is irrelevant. This arises from the fact that the closed models are also finite in the time from initial expansion to final collapse. This time difference, expressed in terms of τ rather than t, is $\tau = 2\pi R$, which shows that a signal can propagate around the universe at most once in the age of the universe. The only question which arises concerns the field at the point on the model opposite the charge at a time πR later than the charge which generates the field. However, the arguments used above still apply. Only in the highly symmetric case would one expect the rays to focus to a point, enabling one to cut off the field by assuming the existence of an opposite charge at that point. In general one would expect the field to propagate continuously until the universe collapses. Therefore again we accept contributions from the source at all retarded times which are inside the age of the universe.

ACKNOWLEDGMENT

The author wishes to thank Dr. Amnon Katz for several stimulating discussions.

[12] The potential for an arbitrary static charge distribution is found to be $A_0 = \Sigma_i q_i \cot \Psi_i(1 - \Psi_i/\pi)$, where $\Psi_i = \Psi(x, x_i)$, $\Sigma_i q_i = 0$, and where there are no image charges.

Involutional Matrices Based on the Representation Theory of $GL(2)$*

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(Received 17 December 1968)

Involutional matrices $M(a, b, c)$ with three arbitrary parameters are introduced, based on a matrix representation $M(R)$ of the linear homogeneous transformation $R \in GL(2)$. Symmetry properties, eigenvalues, and recursion formulas for the representation $M(R)$ are obtained and specialized to the involutional matrices $M(a, b, c)$. A set of special involutional matrices $A(\xi)$, $B(\xi)$, $C(\xi)$, and $E(\xi)$ with one arbitrary parameter ξ are introduced as special cases of $M(a, b, c)$. Their relations are discussed.

1. INTRODUCTION

The purpose of the present work is to study the mathematical properties of involutional matrices which are the solutions of the simple quadratic equation

$$x^2 = \text{const} \times \mathbf{1},$$

where $\mathbf{1}$ is the unit matrix. It is somewhat surprising that this simple looking problem has a deep root in various problems of mathematical physics. Well-known examples of involutional matrices are the Pauli spin matrices.

To illustrate the nature of the problem further, we give two additional examples of involutional matrices $A(\xi)$ and $B(\xi)$ with one arbitrary parameter ξ which the author has introduced in the recent work[1] on the dynamical properties of the Ising lattice. The definitions of these matrices are given by the generating equations

$$(1 + \xi y)^{q-\nu}(1 - y)^{\nu} = \sum_{\mu=0}^{q} A(\xi)_{\nu\mu} y^{\mu}, \tag{1.1}$$

$$(\xi - y)^{\nu} = \sum_{\mu=0}^{\nu} B(\xi)_{\nu\mu} y^{\mu}, \quad \nu = 0, 1, 2, \cdots, q, \tag{1.2}$$

where q is an integer. By the repeated use of these definitions one can easily show that these $(q + 1) \times (q + 1)$ matrices in fact satisfy the involutional relations

$$[A(\xi)]^2 = (1 + \xi)^q \mathbf{1}, \tag{1.3}$$

$$[B(\xi)]^2 = \mathbf{1}. \tag{1.4}$$

These matrices describe the magnetic susceptibilities and the Fisher's algebraic transformation[1,2] of spin–spin correlation of the regular Ising lattice with the coordination number q. It has been shown[1] that the matrix element $A(\xi)_{\nu\mu}$ is closely related to the Jacobi polynomial with the argument $(1 - \xi)/(1 + \xi)$ [see Eqs. (3.12) and (3.21)]. Equation (1.2) which defines the matrix $B(\xi)$ is simply a binomial expansion. An interesting special case of the matrix $A(\xi)$ arises in the Fourier expansion of the following trigonometric function:

$$\cos^{q-\nu}\theta \sin^{\nu}\theta = i^{-2}2^{-q} \sum_{\mu=0}^{q} a_{\nu\mu} e^{i(q-2\mu)\theta}, \tag{1.5}$$

where $a_{\nu\mu} = A\,(\xi = 1)_{\nu\mu}$. We may note here that when $\nu > q$, the right-hand side of Eq. (1.1) becomes an infinite series. Accordingly, the matrix $A(\xi)$ [and also $B(\xi)$ for $\nu < 0$] could be considered as a $\infty \times \infty$ matrix. For further properties of these matrices and their relations the reader is referred to the previous work.[1]

Now we shall return to the general discussion on the solutions of the simple quadratic equation. The one-dimensional solution is trivial. The two-dimensional solution is simply a traceless matrix I with three arbitrary parameters

$$I = \begin{pmatrix} a & b \\ c & -a \end{pmatrix},$$

except for trivial constant matrices. If we regard this matrix I as an element of the general linear homogeneous transformation group in two dimensions, the matrix representation of I by means of a basis set of qth degree homogeneous polynomials in two variables yields a $(q + 1) \times (q + 1)$ involutional matrix $M(I) \equiv M(a, b, c)$ with three arbitrary parameters. Obviously this process of obtaining the higher-dimensional involutional matrix from the lower-dimensional one must apply to the general n-dimensional solution. However, we shall limit the problem to the two-dimensional solution except for giving only a brief discussion on the characteristic relation between the involutional transformation in $GL(n)$ and its representation.

For explicit construction of the representation of $GL(2)$ we shall choose the representation which is the transpose inverse of the ordinary representation

* This work was supported in part by the National Aeronautics and Space Administration through Sustaining University Program Grant GNR 18-002-005 with the University of Louisville.

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[1] Shoon K. Kim, J. Math. Phys. **9**, 1705 (1968).

[2] M. E. Fisher, Phys. Rev. **113**, 969 (1959).

originally due to Wigner.[3,4] The reason is that the present choice yields a direct correlation between the symmetry properties of the group element and its representation. According to this representation the matrices $A(\xi)$ and $B(\xi)$ are given by $M(1, \xi, 1)$ and $M(0, \xi, 1)$, respectively. Depending upon the ranges of the values of ξ, we shall find it convenient to introduce two additional involutional matrices $C(\xi)$ $[= M(1, \xi, 0)]$ and $E(\xi)$ $[= M(\xi, 1, 1)]$. The relations between these will be discussed.

The representation $M(R)$ of the general homogeneous linear transformation $R = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ in two dimensions $GL(2)$ has four arbitrary parameters a, b, c, and d. It is instructive to show that the representation $M(R)$ is completely characterized by the involutional matrix with a single parameter A ($\xi = -bc/ad$) multiplied by a simple product of a, c, and d [see Eq. (3.13)]. Accordingly the study of one parametric involutional matrix carries most of the essential characteristics of the four parametric representations of $R \in GL(2)$. A simple exemplification of this point is the fact that the matrix representation $M[I(\theta)]_{\nu\mu}$ of an involution $I(\theta)$ which is an improper rotation by an angle θ in two dimensions is related to the representation $M[R(\theta)]_{\nu\mu}$ of pure rotation $R(\theta) \in SO(2)$ by a factor $(-1)^{\nu}$ [see Eq. (3.17)].

Guided by the relation between $A(\xi)$ and $M(R)$ we shall extend the previous work on the eigenvalue problem and the symmetry properties of $A(\xi)$ to the corresponding problem of $M(R)$ and then specialize the results for the involutional matrices $M(a, b, c)$. To facilitate the actual construction of these matrices, we shall derive the complete sets of the recursion formulas for the matrices $M(R)$, $A(\xi)$, $B(\xi)$, $C(\xi)$, and $E(\xi)$. As we have shown in the previous work,[1] the actual matrix form of $A(\xi)$ is needed in the description of the magnetic susceptibility of the Ising model. We shall also investigate the integral orthogonal properties of $A(\xi)$ and $E(\xi)$ by means of the corresponding properties of the Jacobi polynomials. Since so much work has been done on $GL(n)$, the author apologizes in advance for not being able to give detailed bibliography.[3]

2. A REPRESENTATION OF INVOLUTIONAL TRANSFORMATION IN $GL(n)$

We shall give a brief preparation for the later sections. Suppose that we have a set of p functions $F_{\nu}(\mathbf{r})$, $\nu = 1, 2, \cdots, p$, of a vector $\mathbf{r} = (x_1, x_2, \cdots, x_n)$ in a n-dimensional space which serves as a basis for a representation of the group of linear homogeneous transformations R in the n-dimensional space $GL(n)$. The representation $M(R)$ may be defined by

$$F_{\nu}(R\mathbf{r}) = \sum_{\mu=1}^{p} M(R)_{\nu\mu} F_{\mu}(\mathbf{r}) \tag{2.1}$$

for all R in $GL(n)$. According to this definition, the representation $M(QR)$ of two successive transformations Q, R is given by the equation

$$F_{\nu}(QR\mathbf{r}) = \sum_{\mu=1}^{p} M(QR)_{\nu\mu} F_{\mu}(\mathbf{r}), \tag{2.2}$$

which leads to

$$M(QR) = M(Q)M(R). \tag{2.3}$$

We note here that the present matrix representation $M(R)$ is chosen differently from the conventional representation in mathematical physics due to Wigner[4] and others[3]; the latter is the inverse transpose of the present one [see Eq. (5.13)]. As we shall see later, the present choice is particularly convenient in the discussion of the symmetry property of $M(R)$ in the sense that the symmetry property of R is directly reflected to that of $M(R)$. We note also that, as far as the definition (2.1) and the group property (2.3) are concerned, singular transformations are not excluded, since inverse transformation does not appear in the definition in contrast with the conventional representation.[3,4]

For our present purpose we take a complete set of linearly independent qth degree homogeneous polynomials in n variables $(x_1, \cdots, x_n)$ as the basis set $\{F_{\nu}(\mathbf{r})\}$. Then the dimension of the representation of $GL(n)$ is given by

$$p = \binom{q + n - 1}{q} \tag{2.4}$$

and the representation $M(R)$ is irreducible. By definition, the basis function $F_{\nu}(\mathbf{r})$ satisfies the Euler condition,

$$F_{\nu}(\lambda\mathbf{r}) = \lambda^{q} F_{\nu}(\mathbf{r}), \quad \nu = 1, 2, \cdots, p. \tag{2.5}$$

Accordingly, the representation satisfies

$$M(\lambda R) = \lambda^{q} M(R), \quad R \in GL(n). \tag{2.6}$$

Obviously, the representation is one-to-q, since, for $\lambda = \exp(2\pi ik/q)$, $k = 1, 2, \cdots, q$, the right-hand side of Eq. (2.6) equals $M(R)$. In the group theory,[5] $M(R)$ is said to be an invariant matrix of the matrix R.

[3] For reviews, see M. Hamermesh, *Group Theory and its Application to Physical Problems* (Addison-Wesley Publ. Co., Inc., Reading, Mass., 1962); *Quantum Theory of Angular Momentum*, L. C. Biedenharn and H. Van Dam, Eds. (Academic Press Inc., New York, 1965).

[4] E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959).

[5] D. E. Littlewood, *The Theory of Group Characters and Matrix Representations of Groups* (Clarendon Press, Oxford, England, 1950), 2nd ed.

Now if we take $R = \mathbf{1}$ where $\mathbf{1}$ is the identical transformation, we obtain

$$M(\lambda\mathbf{1}) = \lambda^q\mathbf{1}. \tag{2.7}$$

Therefore, if I is an involutional transformation in $GL(n)$,

$$I^2 = \lambda\mathbf{1}, \tag{2.8}$$

then its p-dimensional representation $M(I)$ is also involutional and satisfies

$$[M(I)]^2 = \lambda^q\mathbf{1}. \tag{2.9}$$

Since the representation is irreducible, $M(I)$ is involutional only when I is involutional. This equation (2.9) is the basic equation for the present work. In the following section we shall introduce the basis function explicitly and study the properties of the representation $M(I)$ of the involutional transformation I in $GL(2)$.

3. REPRESENTATION OF AN INVOLUTIONAL TRANSFORMATION IN $GL(2)$

We take the following form for the complete set of qth-degree homogeneous polynomials in two variables x and y,

$$F_\nu(\mathbf{r}) = x^{q-\nu}y^\nu, \quad \nu = 0, 1, 2, \cdots, q. \tag{3.1}$$

The linear homogeneous transformation R in two dimensions is given by a 2×2 matrix

$$R = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in GL(2), \tag{3.2}$$

where a, b, c, and d are arbitrary parameters. Then, from Eq. (2.1) we obtain the $(q+1)$-dimensional representation $M(R)$ by

$$F_\nu(R\mathbf{r}) = (ax + by)^{q-\nu}(cx + dy)^\nu = \sum_{\mu=0}^{q} M(R)_{\nu\mu}F_\mu(\mathbf{r}). \tag{3.3}$$

Obviously, $M(R)$ reduces to R when $q = 1$. For later convenience we write down the explicit form of $M(R)$,

$$M(R)_{\nu\mu} = a^{q-\nu-\mu}b^\mu c^\nu \sum_k \binom{\nu}{k}\binom{q-\nu}{\mu-k}\left(\frac{ad}{bc}\right)^k, \tag{3.4}$$

where the limits of summation over k is given by the conditions that the binomial coefficients do not vanish or blow up. In the discussion of the integral properties and symmetry properties of the matrix $M(R)$, it is useful to express the matrix elements in terms of the hypergeometric functions,[6]

$$\begin{aligned} M(R)_{\nu\mu} &= a^{q-\nu-\mu}b^\mu c^\nu \binom{q-\nu}{\mu} \\ &\quad \times {}_2F_1\left(-\nu, -\mu; q-\nu-\mu+1, \frac{ad}{bc}\right) \\ &= a^{q-\nu}c^{\nu-\mu}d^\mu \binom{\nu}{\mu} \\ &\quad \times {}_2F_1\left(\nu-q, -\mu; \nu-\mu+1, \frac{bc}{ad}\right), \end{aligned} \tag{3.5}$$

where $q - \nu - \mu \geq 0$ for the first expression and $\nu \geq \mu$ for the second. These expressions are valid even when q and ν are not integers provided that the $|ad/bc| < 1$ for the first and $|bc/ad| < 1$ for the second expression. However, we shall not make this generalization.

Now if we exclude constant matrices, the most general involutional transformation in two dimensions is given by

$$I(a, b, c) = \begin{pmatrix} a & b \\ c & -a \end{pmatrix}, \quad [I(a, b, c)]^2 = (a^2 + bc)\mathbf{1}, \tag{3.6}$$

where a, b, and c are arbitrary parameters. This is obtained by the nontrivial solution of the quadratic equation (trivial solutions mean constant matrices):

$$R^2 = \begin{pmatrix} a^2 + bc & (a+d)b \\ (a+d)c & d^2 + bc \end{pmatrix} = \text{const} \times \mathbf{1}.$$

We may state that nontrivial 2×2 involutional matrices are traceless. We shall see later, however, that the matrix representations of $I(a, b, c)$ are not always traceless, depending upon the dimension of the representation. From Eqs. (2.8) and (2.9) we have for the $(q+1)$-dimensional representation $M(a, b, c)$ of $I(a, b, c)$:

$$M(a, b, c) \equiv M\left[\begin{pmatrix} a & b \\ c & -a \end{pmatrix}\right], \tag{3.7}$$

$$[M(a, b, c)]^2 = (a^2 + bc)^q\mathbf{1}.$$

The explicit form of this matrix representation is obtained simply by putting $d = -a$ in Eqs. (3.4) and (3.5).

It is now a simple matter to understand why the matrices $A(\xi)$ and $B(\xi)$ which we have introduced in the introduction are involutional. In fact, comparing

[6] *National Bureau of Standards, Applied Mathematical Series, Vol. 55: Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun, Eds. (National Bureau of Standards, Washington, D.C., 1964), p. 556.

Eqs. (1.1) and (1.2) with Eq. (3.3) we obtain

$$A(\xi) = M\left[\begin{pmatrix} 1 & \xi \\ 1 & -1 \end{pmatrix}\right], \quad B(\xi) = M\left[\begin{pmatrix} 1 & 0 \\ \xi & -1 \end{pmatrix}\right], \tag{3.8}$$

which are certainly the representations of traceless matrices. Depending upon the ranges of values which the parameter ξ takes, we may find it more convenient in application to introduce the following matrices:

$$C(\xi) = M\left[\begin{pmatrix} 1 & \xi \\ 0 & -1 \end{pmatrix}\right], \quad E(\xi) = M\left[\begin{pmatrix} \xi & 1 \\ 1 & -\xi \end{pmatrix}\right], \tag{3.9}$$

which satisfy

$$[C(\xi)]^2 = \mathbf{1}, \quad [E(\xi)]^2 = (1 + \xi^2)^q \mathbf{1}.$$

We have saved the symbol D for the conventional representation due to Wigner.[3,4] The generating equations of these matrices are

$$(1 + \xi y)^{q-\nu}(-y)^\nu = \sum_{\mu=\nu}^{q} C(\xi)_{\nu\mu} y^\mu, \tag{3.10}$$

$$(\xi + y)^{q-\nu}(1 - \xi y)^\nu = \sum_{\mu=0}^{q} E(\xi)_{\nu\mu} y^\mu. \tag{3.11}$$

Comparing the generating equations (1.1), (1.2), (3.10), and (3.11), we obtain the following relations:

$$\binom{q}{\nu} C(\xi)_{\nu\mu} = \binom{q}{\mu} B(\xi)_{\mu\nu}, \tag{3.12}$$

$$E(\xi)_{\nu\mu} = \xi^{q+\mu-\nu} A(\xi^{-2})_{\nu\mu}.$$

It is also possible to express the representation $M(R)$ of the general linear transformation $R \in GL(2)$ in terms of $A(\xi)$:

$$M\left[\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right]_{\nu\mu} = a^{q-\nu} c^{\nu-\mu} (-d)^\mu A\left(-\frac{bc}{ad}\right)_{\nu\mu}. \tag{3.13}$$

The general nature and the usefulness of the involutional matrix $A(\xi)$ lie in this formula. Further important properties of the matrices $A(\xi)$ and $B(\xi)$ are given in the previous work.[1]

In order to have a further understanding of the involutional transformation, we put $a^2 + bc = 1$ in Eq. (3.6) and obtain an involution defined by

$$I(b, c) = \begin{pmatrix} (1 - bc)^{\frac{1}{2}} & b \\ c & -(1 - bc)^{\frac{1}{2}} \end{pmatrix}, \tag{3.14}$$

which satisfies $[I(bc)]^2 = 1$ for arbitrary values of b and c. Since $\det I(b, c) = -1$, nontrivial involutions do not belong to $SL(2)$. By means of a similarity transformation with the matrix T defined by

$$T = \begin{pmatrix} 1 & 0 \\ 0 & (b/c)^{\frac{1}{2}} \end{pmatrix},$$

we can reduce $I(bc)$ into a symmetric orthogonal matrix which is still an involution

$$I(\theta) = TI(b, c)T^{-1} = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}, \tag{3.15}$$

where we have set $(bc)^{\frac{1}{2}} = \sin\theta$. Obviously, for a real value of θ, the involution $I(\theta)$ describes an improper rotation, a rotation $R(\theta)$ of the coordinate system (x, y) by an angle θ followed by the reflection σ_x in the x axis

$$I(\theta) = \sigma_x R(\theta), \tag{3.16}$$

where

$$\sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad R(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}.$$

If we give the matrix representation of Eq. (3.16), we obtain

$$M[I(\theta)]_{\nu\mu} = (-1)^\nu M[R(\theta)]_{\nu\mu}, \tag{3.17}$$

which connects the representation of an involution with the representation of the pure rotation. A trivial but useful conclusion is that the right-hand side is also an involution.

We can easily generalize Eq. (3.15) for the case of $I(a, b, c)$ when $a^2 + bc \neq 1$ to obtain

$$I(\theta) = T \frac{I(a, b, c)}{(a^2 + bc)^{\frac{1}{2}}} T^{-1}, \tag{3.18}$$

where T is the same as before and $\tan^2\theta = bc/a^2$. Giving the representation of this equation we obtain

$$M[I(\theta)]_{\nu\mu} = (a^2 + bc)^{-\frac{1}{2}q} (b/c)^{\frac{1}{2}(\nu-\mu)} M(a, b, c)_{\nu\mu}. \tag{3.19}$$

Using Eq. (3.13) and the second equation of Eq. (3.12) we can express the right-hand side of this equation in terms of $A(\xi)$ and $E(\xi)$ as

$$\begin{aligned} M[I(\theta)]_{\nu\mu} &= \cos^{q-\nu+\mu}\theta \sin^{\nu-\mu}\theta A(\tan^2\theta)_{\nu\mu} \\ &= \sin^q\theta E(\cot\theta)_{\nu\mu}. \end{aligned} \tag{3.20}$$

Equations (3.18)–(3.20) connect the properties of involutional matrices with the well-known properties of the representation of the two-dimensional pure rotation group. For example, we can expect the integral orthogonal properties of the polynomials of ξ, $A(\xi)_{\nu\mu}$, and $E(\xi)_{\nu\mu}$ from the orthogonality theorem of $M(R(\theta))_{\nu\mu}$ which we shall discuss in the following.

Using the first of Eqs. (3.5) we can express $E(\xi)_{\nu\mu}$ in terms of the hypergeometric function and compare with the definition of the Jacobi polynomial[7] expressed in terms of the hypergeometric function to obtain

$$E^{(q)}_{\nu\mu}(\eta) = \eta^\alpha (1 + \eta^2)^n P_n^{(\alpha,\beta)}((1 - \eta^2)/(1 + \eta^2)), \tag{3.21}$$

where we have denoted q dependence of $E(\eta)$ explicitly and

$$\alpha = q - \nu - \mu > -1, \quad \beta = \nu - \mu > -1, \quad n = \mu.$$

[7] See Ref. 6, p. 773.

The Jacobi polynomials satisfy the orthogonal theorem,[7]

$$J_{nm}^{(\alpha,\beta)} = \int_{-1}^{1} (1-x)^{\alpha}(1-x)^{\beta} P_n^{(\alpha,\beta)}(x) P_m^{(\alpha,\beta)}(x)\, dx$$
$$= \delta_{nm} \frac{2^{\gamma+1}}{\gamma+2n+1} \binom{\gamma+2n}{n} \Big/ \binom{\gamma+2n}{\beta+n}, \tag{3.22}$$

where δ_{nm} is the Kronecker delta and

$$\gamma = \alpha + \beta.$$

Substituting Eq. (3.21) into Eq. (3.22) and using the second equation of Eq. (3.12) and Eq. (3.20) we obtain

$$J_{nm}^{(\alpha,\beta)} = 2^{\gamma+2} \int_0^{\infty} \frac{\eta}{(1+\eta^2)^{\gamma+n+m+2}} E_{\beta+n,n}^{(\gamma+2n)}(\eta) E_{\beta+m,m}^{(\gamma+2m)}(\eta)\, d\eta$$
$$= 2^{\gamma+1} \int_0^{\infty} \frac{\xi^{\beta}}{(1+\xi)^{\gamma+n+m+2}} A_{\beta+n,n}^{(\gamma+2n)}(\xi) A_{\beta+m,m}^{(\gamma+2m)}(\xi)\, d\xi$$
$$= 2^{\gamma} \int_0^{\pi} \bar{M}_{\beta+n,n}^{(\gamma+2n)}(\tfrac{1}{2}\theta) \bar{M}_{\beta+m,m}^{(\gamma+2m)}(\tfrac{1}{2}\theta) \sin\theta\, d\theta, \tag{3.23}$$

where the matrix $\bar{M}(\frac{1}{2}\theta)$ equals either $M[I(\frac{1}{2}\theta)]$ or $M[R(\frac{1}{2}\theta)]$. We can simplify these equations further if we introduce the "symmetrized representation" $S(\frac{1}{2}\theta)$ by a similarity transformation of $\bar{M}(\frac{1}{2}\theta)$:

$$\bar{S}_{\nu\mu}^{(q)}(\tfrac{1}{2}\theta) = \binom{q}{\nu}^{\frac{1}{2}} \bar{M}_{\nu\mu}^{(q)}(\tfrac{1}{2}\theta) \binom{q}{\mu}^{-\frac{1}{2}}. \tag{3.24}$$

The properties of this representation will be discussed extensively in connection with the symmetry properties of the representation $M(R)$. Substituting Eq. (3.24) into the last expression of Eq. (3.23) we obtain

$$\int_0^{\pi} \bar{S}_{\beta+n,n}^{(\gamma+2n)}(\tfrac{1}{2}\theta) \bar{S}_{\beta+m,m}^{(\gamma+2m)}(\tfrac{1}{2}\theta) \sin\theta\, d\theta$$
$$= 2\delta_{nm}/(\gamma+2n+1). \tag{3.25}$$

As may become clearer later when we establish the relation (Eq. 5.17) between $S(u)$ and the Wigner's $\mathfrak{D}^j(u)$ function[4] where u is a unitary matrix, Eq. (3.25) is nothing but the basic orthogonal theorem in the double-valued representation of the three-dimensional rotation group.

4. EIGENVALUES OF $M(R)$ AND $M(I)$

First we shall calculate the eigenvalues of the matrix representation $M(R)$ of the general linear transformation R in $GL(2)$ defined by Eq. (3.2), then specialize the results for the representation of involutional transformation defined by Eq. (3.6). The calculation is based on the following simple theorem.

Theorem 1: If R is a triangular matrix, then its matrix representation $M(R)$ is also triangular in shape similar to R.

The proof is trivial. Suppose one of the matrix elements b of R be zero so that R becomes a triangular matrix R_t defined by

$$R_t = \begin{pmatrix} a & 0 \\ c & d \end{pmatrix}. \tag{4.1}$$

Then from Eq. (3.3) we obtain

$$a^{q-\nu}(c+dy)^{\nu} = \sum_{\mu=0}^{\nu} M_{\nu\mu} y^{\mu}. \tag{4.2}$$

Accordingly, $M_{\nu\mu} = 0$ for $\mu > \nu$. In the analogous manner, whenever one of the matrix elements of R becomes zero, the nonzero matrix elements of its representation $M(R)$ form a triangle in shape equivalent to R.

According to the well-known theorem, it is always possible to transform any arbitrary square matrix into a triangular matrix by a suitable unitary transformation. Let U be such a unitary matrix which transforms R into a triangular matrix R_t,

$$U^{-1}RU = \begin{pmatrix} \epsilon_1 & 0 \\ \zeta & \epsilon_2 \end{pmatrix} \equiv R_t, \tag{4.3}$$

where ζ is a constant and ϵ_1 and ϵ_2 are the eigenvalues of R. According to Theorem 1 the representation $M(R_t)$ is also triangular and thus its diagonal elements are the eigenvalues of $M(R)$. Substituting R_t in Eq. (3.3) we obtain the representation $M(R_t)$,

$$M(R_t)_{\nu\mu} = \binom{\nu}{\mu} \zeta^{\nu-\mu} \epsilon_1^{q-\nu} \epsilon_2^{\nu}, \quad \zeta \neq 0,$$
$$= \delta_{\nu\mu} \epsilon_1^{q-\nu} \epsilon_2^{\nu}, \qquad \zeta = 0, \tag{4.4}$$

where $\delta_{\nu\mu}$ is Kronecker's delta. Therefore, the eigenvalues of $M(R)$ are given by

$$\epsilon_1^{q-\nu} \epsilon_2^{\nu}, \quad \nu = 0, 1, 2, \cdots, q. \tag{4.5}$$

The determinant of the matrix $M(R)$ is given by

$$\det M(R) = \prod_{\nu=0}^{q} \epsilon_1^{q-\nu} \epsilon_2^{\nu} = (\epsilon_1 \epsilon_2)^{\frac{1}{2}q(q+1)} = \Delta^{\frac{1}{2}q(q+1)}, \tag{4.6}$$

where $\Delta = ad - bc$ the determinant of the matrix R. The trace of $M(R)$ is given by

$$\operatorname{Tr} M(R) = \sum_{\nu=0}^{q} \epsilon_1^{q-\nu} \epsilon_2^{\nu}$$
$$= (\epsilon_1^{q+1} - \epsilon_2^{q+1})/(\epsilon_1 - \epsilon_2), \quad \epsilon_1 \neq \epsilon_2,$$
$$= (q+1)\epsilon_1^{q}, \qquad \epsilon_1 = \epsilon_2. \tag{4.7}$$

We shall apply these general results to the representation of the involutional transformation $I(a, b, c)$ defined by Eq. (3.6). From the definition, the eigenvalues of $I(a, b, c)$ are $\pm\epsilon$, where

$$\epsilon = (a^2 + bc)^{\frac{1}{2}}, \tag{4.8}$$

and the determinant is given by

$$\det I(a, b, c) = -\epsilon^2. \tag{4.9}$$

Accordingly, from Eq. (4.5) its representation $M(a, b, c)$ has only two eigenvalues $\pm\epsilon^q$ and its

determinant and trace are

$$\det M(a, b, c) = (-\epsilon^2)^{\frac{1}{2}q(q+1)},$$
$$\operatorname{Tr} M(a, b, c) = \epsilon^q, \quad q = \text{even}, \qquad (4.10)$$
$$= 0, \quad q = \text{odd}.$$

Therefore, when q is even, the degeneracy of the eigenvalue ϵ^q is larger by one than that of $-\epsilon^q$. We may note here that the trace of a nontrivial 2×2 involutional matrix is always zero but the trace of its representation is not necessarily zero. We also note that all these properties of $M(a, b, c)$ are described by a single parameter ϵ. This is not surprising because of the following discussion.

If we restrict ourselves to the eigenvalue problem of involutional matrices from the beginning we can handle the problem more generally. Let $M(I)$ be the p-dimensional representation of an involutional transformation I in n dimensions defined by Eq. (2.8). Then rewriting Eq. (2.9) we obtain

$$M(I)X_\pm = \pm\lambda^{\frac{1}{2}q}X_\pm, \quad X_\pm = M(I) \pm \lambda^{\frac{1}{2}q}\mathbf{1}, \qquad (4.11)$$

where $+$ $(-)$ sign should be taken for $X_+(X_-)$. Therefore, the eigenvalues of $M(I)$ are $\pm\lambda^{\frac{1}{2}q}$ and the corresponding eigenvectors are given by the column vectors of $X_\pm$. At least half of these eigenvectors are redundant. We can also write down the square of the determinant $M(I)$,

$$[\det M(I)]^2 = \lambda^{qp}, \qquad (4.12)$$

where p is given by Eq. (2.4) and, in particular, $p = q + 1$ for $I \in GL(2)$.

5. SYMMETRY PROPERTIES OF $M(R)$, $S(R)$, AND $M(I)$

To obtain the symmetry properties of $M(I)$ we first study the symmetry properties of the representation $M(R)$ for the general linear transformation R in two dimensions, many of which may have been known. The most obvious symmetry property of $M(R)$ arises from the fact that $F_\nu(\mathbf{r}) = x^{q-\nu}y^\nu$ is $(q - \nu)$th degree in x and νth degree in y. With this in mind, inspection of the generating equation (3.3) for $M(R)$ yields

$$\begin{aligned} M\left[\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right]_{\nu\mu} &= \lambda^{\nu-q} M\left[\begin{pmatrix} \lambda a & \lambda b \\ c & d \end{pmatrix}\right]_{\nu\mu} \\ &= \lambda^{-\nu} M\left[\begin{pmatrix} a & b \\ \lambda c & \lambda d \end{pmatrix}\right]_{\nu\mu} \\ &= \lambda^{\mu-q} M\left[\begin{pmatrix} \lambda a & b \\ \lambda c & d \end{pmatrix}\right]_{\nu\mu} \\ &= \lambda^{-\mu} M\left[\begin{pmatrix} a & \lambda b \\ c & \lambda d \end{pmatrix}\right]_{\nu\mu} \\ &= \lambda^{-q} M\left[\begin{pmatrix} \lambda a & \lambda b \\ \lambda c & \lambda d \end{pmatrix}\right]_{\nu\mu}. \end{aligned} \qquad (5.1)$$

Hereafter we refer to these as the Euler relations for $M(R)$. More frequently than not, we use these equations for $\lambda = -1$, in which case combination of the above equalities yields two additional properties,

$$\begin{aligned} M\left[\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right]_{\nu\mu} &= (-1)^{\nu+\mu} M\left[\begin{pmatrix} a & -b \\ -c & d \end{pmatrix}\right]_{\mu\nu} \\ &= (-1)^{q+\nu+\mu} M\left[\begin{pmatrix} -a & b \\ c & -d \end{pmatrix}\right]_{\nu\mu}. \end{aligned} \qquad (5.2)$$

Further symmetries of the matrix $M(R)$ arises from the fact that the basis function $F_\nu(\mathbf{r}) = x^{q-\nu}y^\nu$ is invariant with respect to the simultaneous interchanges $q - \nu \rightleftarrows \nu$ and $x \rightleftarrows y$. Applying this property into the generating equation (3.3) of $M(R)$ we obtain

$$\begin{aligned} M\left[\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right]_{\nu\mu} &= M\left[\begin{pmatrix} c & d \\ a & b \end{pmatrix}\right]_{q-\nu,\mu} \\ &= M\left[\begin{pmatrix} b & a \\ d & c \end{pmatrix}\right]_{\nu,q-\mu} = M\left[\begin{pmatrix} d & c \\ b & a \end{pmatrix}\right]_{q-\nu,q-\mu}. \end{aligned} \qquad (5.3)$$

These equations mean the following. We regard the matrices $M(R)$ and R as rectangulars (not squares) whose edges are parallel to the rows and columns of the matrices. The set of symmetry operations $\mathbf{P}_2$ which leaves the rectangular invariant forms the dihedral group $\mathbf{D}_2$ which consists of three 2-fold axes of rotation. Then the above equations (5.3) are written formally as

$$M(\mathbf{P}_2 R) = \mathbf{P}_2 M(R), \quad \mathbf{P}_2 \in \mathbf{D}_2. \qquad (5.4)$$

More important symmetry properties of $M(R)$ arise from the symmetry of the following bilinear form in x and y:

$$\sum_{\nu=0}^{q}\sum_{\mu=0}^{q} d^q \left(\frac{bx}{d}\right)^\nu M(R)_{\nu\mu}\left(\frac{cy}{d}\right)^\mu = [ad + bc(x + y + xy)]^q, \qquad (5.5)$$

where we have used Eq. (3.3). Obviously the right-hand side of the equation is symmetric with respect to (x, y) or (b, c) or (a, d). Therefore, we obtain the following theorem:

Theorem 2: The expression $\binom{q}{\nu} d^{q-\nu-\mu} b^\nu c^\mu M[\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)]_{\nu\mu}$ is invariant for interchanges of two variables (ν, μ) or (b, c) or (a, d).

By means of this theorem, if we perform the simultaneous interchanges $(\nu \rightleftarrows \mu)$ and $(b \rightleftarrows c)$ for the expression defined in the theorem, we obtain

$$\binom{q}{\nu} M(R)_{\nu\mu} = \binom{q}{\mu} M(\tilde{R})_{\mu\nu}, \qquad (5.6)$$

where $\tilde{R}$ is the transpose of R. Accordingly, if we introduce a matrix defined by

$$S(R)_{\nu\mu} = \binom{q}{\nu}^{\frac{1}{2}} M(R)_{\nu\mu} \binom{q}{\mu}^{-\frac{1}{2}}, \tag{5.7}$$

it satisfies

$$\tilde{S}(R) = S(\tilde{R}). \tag{5.8}$$

Since $S(R)$ and $M(R)$ are related by a similarity transformation, $S(R)$ is also a representation of $R \in GL(2)$. In fact, $S(R)$ is generated by the normalized basis function $f_\nu(\mathbf{r}) = x^{q-\nu}y^\nu/[(q-\nu)!\,\nu!]^{\frac{1}{2}}$ which is well known in the representation theory of the unitary groups in two dimensions[3,4]

$$f_\nu(R\mathbf{r}) = \sum_\mu S(R)_{\nu\mu} f_\mu(\mathbf{r}). \tag{5.9}$$

We call this representation the symmetrized representation. Obviously, $S(R)$ satisfies all the symmetry properties of $M(R)$ given by Eqs. (5.1), (5.2), and (5.3). If we combine Eqs. (5.4) and (5.8) we may write the symmetry properties of $S(R)$ formally as follows,

$$S(\mathbf{P}_4 R) = P_4 S(R), \quad \mathbf{P}_4 \in \mathbf{D}_4, \tag{5.10}$$

where $\mathbf{P}_4$ is a symmetry operation which leaves a square invariant, regarding the matrices $S(R)$ and R as squares. The set of symmetry operations forms the dihedral group $\mathbf{D}_4$. We can write Eq. (5.10) explicitly as follows:

$$\begin{aligned} S\left[\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right]_{\nu\mu} &= S\left[\begin{pmatrix} c & d \\ a & b \end{pmatrix}\right]_{q-\nu,\mu} \\ &= S\left[\begin{pmatrix} b & a \\ d & c \end{pmatrix}\right]_{\nu,q-\mu} = S\left[\begin{pmatrix} d & c \\ b & a \end{pmatrix}\right]_{q-\nu,q-\mu} \\ &= S\left[\begin{pmatrix} a & c \\ b & d \end{pmatrix}\right]_{\mu\nu} = S\left[\begin{pmatrix} c & a \\ d & b \end{pmatrix}\right]_{\mu,q-\nu} \\ &= S\left[\begin{pmatrix} b & d \\ a & c \end{pmatrix}\right]_{q-\mu,\nu} = S\left[\begin{pmatrix} d & b \\ c & a \end{pmatrix}\right]_{q-\mu,q-\nu}. \end{aligned} \tag{5.11}$$

Before we give further discussions on the symmetry properties of $M(R)$ and $S(R)$, we discuss a couple of elementary but important applications of these symmetry properties. If we combine Eq. (5.8) with the property that $S(R)^* = S(R^*)$, where asterisk denotes the complex conjugate, we can conclude that, if the matrix R is symmetric or Hermitian or orthogonal or unitary, then so is $S(R)$ in each case. This is well known but the present proof is direct and simpler than the proof given by Wigner[4] for the case when R is unitary.

The conventional representation due to Wigner[4] is defined by

$$f_\nu(R^{-1}\mathbf{r}) = \sum_{\mu=0}^{q} f_\mu(\mathbf{r}) D(R)_{\mu\nu}. \tag{5.12}$$

Accordingly, $D(R)$ is given by $S(R)$ as follows:

$$D(R) = \tilde{S}(R^{-1}). \tag{5.13}$$

Since the inverse of R is given by

$$R^{-1} = \frac{1}{\Delta}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}, \quad \Delta = \det R = ad - bc, \tag{5.14}$$

we obtain

$$\begin{aligned} S(R^{-1})_{\nu\mu} &= \Delta^{-q} S\left[\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}\right]_{\nu\mu} \\ &= (-1)^{\nu+\mu}\Delta^{-q} S(R)_{q-\mu,q-\nu}, \end{aligned} \tag{5.15}$$

where we have used Euler's relations (5.1) and (5.2) and the last equality of Eq. (5.11). Accordingly, from Eqs. (5.13), and (5.15) we have

$$D(R)_{\nu\mu} = (-1)^{\nu+\mu}\Delta^{-q} S(R)_{q-\nu,q-\mu}. \tag{5.16}$$

It is obvious that, when $\Delta = 1$, the representations $D(R)$ and $S(R)$ are equivalent. The Wigner function $\mathfrak{D}^j(U)_{m'm}$ with $j = \frac{1}{2}q$ in the double-valued representation of three-dimensional rotation[4] is given by

$$\begin{aligned} \mathfrak{D}^j(U)_{m',m} &= (-1)^{m'+m} D(U)_{j-m',j-m} \\ &= S(U)_{j+m',j+m}, \end{aligned} \tag{5.17}$$

where U is a unitary matrix belonging to $SU(2)$. Note that the suffixes of $S(U)$ are always integers so that half-integral suffix could be preferably avoided by using the representation $S(U)$.

We shall now return to further discussions on the symmetry properties of $M(R)$. Somewhat less elegant but useful symmetry properties of $M(R)$ are obtained by using Euler's relations and Theorem 2 concerning the interchange ($b \rightleftarrows c$) or ($a \rightleftarrows d$). The results are

$$\begin{aligned} M\left[\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right]_{\nu\mu} &= \left(\frac{c}{b}\right)^{\nu-\mu} M\left[\begin{pmatrix} a & c \\ b & d \end{pmatrix}\right]_{\nu\mu} \\ &= \left(\frac{a}{d}\right)^{q-\nu-\mu} M\left[\begin{pmatrix} d & b \\ c & a \end{pmatrix}\right]_{\nu\mu} \\ &= \left(\frac{c}{b}\right)^{\nu-\mu}\left(\frac{a}{d}\right)^{q-\nu-\mu} M\left[\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right]_{q-\nu,q-\mu} \\ &= (ab)^{q-\nu} M\left[\begin{pmatrix} b^{-1} & a^{-1} \\ c & d \end{pmatrix}\right]_{\nu\mu} \\ &= (cd)^{\nu} M\left[\begin{pmatrix} a & b \\ d^{-1} & c^{-1} \end{pmatrix}\right]_{\nu\mu} \\ &= (ab)^{q-\nu}(cd)^{\nu} M\left[\begin{pmatrix} a^{-1} & b^{-1} \\ c^{-1} & d^{-1} \end{pmatrix}\right]_{\nu,q-\mu} \\ &= (ac)^{q-\mu}(bd)^{\mu} M\left[\begin{pmatrix} a^{-1} & b^{-1} \\ c^{-1} & d^{-1} \end{pmatrix}\right]_{q-\nu,\mu}. \end{aligned} \tag{5.18}$$

It is obvious that the symmetrized representation $S(R)$ satisfies all these equations besides Eq. (5.11).

We shall now specialize these symmetry relations for the case of the involutional matrices $M(a, b, c)$ and $S(a, b, c)$, where $M(a, b, c)$ is given by Eq. (3.7) and $S(a, b, c)$ is defined by

$$S(a, b, c) = S\left[\begin{pmatrix} a & b \\ c & -a \end{pmatrix}\right]. \tag{5.19}$$

Because of the restriction $d = -a$, the number of symmetry relations for these reduces. We write down the results as follows:

$$\begin{aligned} M(a, b, c)_{\nu\mu} &= \lambda^{-q} M(\lambda a, \lambda b, \lambda c)_{\nu\mu} \\ &= (-1)^{\nu+\mu} M(a, -b, -c)_{\nu\mu} \\ &= (-1)^{q+\nu+\mu} M(-a, b, c)_{\nu\mu} \\ &= (c/b)^{\nu-\mu} M(a, c, b)_{\nu\mu} \\ &= (-1)^{q-\nu-\mu}(c/b)^{\nu-\mu} M(a, b, c)_{q-\nu,q-\mu} \\ &= (ab)^q(-c/b)^\nu M(a^{-1}, b^{-1}, c^{-1})_{\nu,q-\mu} \\ &= (ac)^q(-b/c)^\mu M(a^{-1}, b^{-1}, c^{-1})_{q-\nu,\mu}. \end{aligned} \tag{5.20}$$

Besides these the matrix $S(a, b, c)$ satisfies

$$S(a, b, c)_{\nu\mu} = S(a, c, b)_{\mu\nu}. \tag{5.21}$$

Since the symmetry properties of $A(\xi)$ have been given in the previous work[1] we shall only give the symmetry properties of $E(\xi) \equiv M(\xi, 1, 1)$,

$$\begin{aligned} E(\xi)_{\nu\mu} &= (-1)^{q+\nu+\mu} E(-\xi)_{\nu\mu} \\ &= (-1)^{q+\nu+\mu} E(\xi)_{q-\nu,q-\mu} \\ &= (-1)^\nu \xi^q E(\xi^{-1})_{\nu,q-\mu} \\ &= (-1)^\mu \xi^q E(\xi^{-1})_{q-\nu,\mu}, \end{aligned} \tag{5.22}$$

and the corresponding symmetrized representation $\hat{E}(\xi) \equiv S(\xi, 1, 1)$ satisfies

$$\hat{E}(\xi)_{\nu\mu} = \hat{E}(\xi)_{\mu\nu}. \tag{5.23}$$

Finally, for the representation $S(\theta) = S[I(\theta)]$ of the two-dimensional involution $I(\theta)$ defined by Eq. (3.15) we have

$$\begin{aligned} S(\theta)_{\nu\mu} = S(\theta)_{\mu\nu} &= (-1)^{q+\nu+\mu} S(\theta)_{q-\nu,q-\mu} \\ &= (-1)^{\nu+\mu} S(-\theta)_{\nu\mu} \end{aligned} \tag{5.24}$$

and

$$\begin{aligned} S(\tfrac{1}{2}\pi - \theta)_{\nu\mu} &= (-1)^\nu S(\theta)_{\nu,q-\mu}, \\ S(\tfrac{1}{2}\pi + \theta)_{\nu\mu} &= (-1)^{q-\mu} S(\theta)_{\nu,q-\mu}, \\ S(\pi - \theta)_{\nu\mu} &= (-1)^{q+\nu+\mu} S(\theta)_{\nu\mu}, \\ S(\pi + \theta)_{\nu\mu} &= (-1)^q S(\theta)_{\nu\mu}. \end{aligned} \tag{5.25}$$

As is well known, analogous equations hold for the representation $S[R(\theta)]$ of the proper rotation $R(\theta)$ in two dimensions. This is seen most easily from the relation

$$S(\theta)_{\nu\mu} = (-1)^\nu S[R(\theta)]_{\nu\mu}, \tag{5.26}$$

because of Eq. (3.17).

6. RECURSION FORMULAS OF $M(R)$ AND INVOLUTIONAL MATRICES

In the derivation of the recursion formulas it is necessary to denote the degree of the basis polynomials of the representation explicitly, thus

$$F_\nu^{(q)}(\mathbf{r}) = x^{q-\nu} y^\nu, \quad \nu = 0, 1, 2, \cdots, q.$$

By definition we have

$$F_\nu^{(q)}(\mathbf{r}) = F_{\nu_1}^{(q_1)}(\mathbf{r}) F_{\nu-\nu_1}^{(q-q_1)}(\mathbf{r}), \quad q_1 \le q, \nu_1 \le \nu. \tag{6.1}$$

Introducing a linear transformation $R \in GL(2)$ in this equation and expanding it by means of Eq.(3.3), we obtain

$$M^{(q)}(R)_{\nu\mu} = \sum_{\mu_1=0}^{\mu} M^{(q_1)}(R)_{\nu_1\mu_1} M^{(q-q_1)}(R)_{\nu-\nu_1,\mu-\mu_1}. \tag{6.2}$$

In the special cases where $q_1 = 1$ or $q_1 = q - 1$, this equation becomes

$$\begin{aligned} M_{\nu\mu}^{(q)} &= a M_{\nu\mu}^{(q-1)} + b M_{\nu,\mu-1}^{(q-1)} \\ &= c M_{\nu-1,\mu}^{(q-1)} + d M_{\nu-1,\mu-1}^{(q-1)}, \end{aligned} \tag{6.3}$$

where we have omitted the argument R for simplicity. Equations (6.3) are particularly useful in obtaining the explicit form of the matrix $M(R)$. Actually these are generalizations of the well-known pyramidal rule for the binomial coefficients

$$\binom{q}{\mu} = \binom{q-1}{\mu} + \binom{q-1}{\mu-1}.$$

In fact, Eqs. (6.3) reduce to this if we set $R = \left(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix}\right)$. Analogous recursion formulas are obtained if we differentiate both sides of the generating equation (3.3) of $M(R)$ with respect to x or y,

$$\begin{aligned} (q - \mu) M_{\nu\mu}^{(q)} &= a(q - \nu) M_{\nu,\mu}^{(q-1)} + c\nu M_{\nu-1,\mu}^{(q-1)}, \\ \mu M_{\nu\mu}^{(q)} &= b(q - \nu) M_{\nu,\mu-1}^{(q-1)} + d\nu M_{\nu-1,\mu-1}^{(q-1)}. \end{aligned} \tag{6.4}$$

The recursion formulas involving the differential coefficients of $M(R)$ are obtained by differentiating the generating equation with respect to a or b or c or d. The results are

$$\begin{aligned} \frac{\partial}{\partial a} M_{\nu,\mu}^{(q)} &= (q - \nu) M_{\nu,\mu}^{(q-1)}, \\ \frac{\partial}{\partial b} M_{\nu,\mu}^{(q)} &= (q - \nu) M_{\nu,\mu-1}^{(q-1)}, \\ \frac{\partial}{\partial c} M_{\nu\mu}^{(q)} &= \nu M_{\nu-1,\mu}^{(q-1)}, \\ \frac{\partial}{\partial d} M_{\nu\mu}^{(q)} &= \nu M_{\nu-1,\mu-1}^{(q-1)}. \end{aligned} \tag{6.5}$$

Repeated uses of these yield the differential equation for $M(R)$:

$$\left(\frac{\partial^2}{\partial a \partial d} - \frac{\partial^2}{\partial b \partial c}\right) M(R) = 0. \tag{6.6}$$

These equations (6.3)–(6.5) form the fundamental set of the recursion formulas.

We can obtain an auxiliary set of recursion formulas which exhibit the various homogeneous dependence of $M(R)$ on the matrix elements a, b, c, and d by applying Euler's theorem on Eq. (5.1):

$$\begin{aligned}
\left(a\frac{\partial}{\partial a} + b\frac{\partial}{\partial b}\right) M^{(q)}_{\nu\mu} &= (q-\nu) M^{(q)}_{\nu\mu}, \\
\left(c\frac{\partial}{\partial c} + d\frac{\partial}{\partial d}\right) M^{(q)}_{\nu\mu} &= \nu M^{(q)}_{\nu\mu}, \\
\left(a\frac{\partial}{\partial a} + c\frac{\partial}{\partial c}\right) M^{(q)}_{\nu\mu} &= (q-\mu) M^{(q)}_{\nu\mu}, \\
\left(b\frac{\partial}{\partial b} + d\frac{\partial}{\partial d}\right) M^{(q)}_{\nu\mu} &= \mu M^{(q)}_{\nu\mu},
\end{aligned} \tag{6.7}$$

and

$$\left(a\frac{\partial}{\partial a} + b\frac{\partial}{\partial b} + c\frac{\partial}{\partial c} + d\frac{\partial}{\partial d}\right) M^{(q)}(R) = q M^{(q)}(R). \tag{6.8}$$

These formulas can be easily obtained by combining the fundamental set (6.3)–(6.5).

Now we shall specialize these formulas for the involutional matrices. The recursion formulas for the general involutional matrices $M(a, b, c)$ are not much simpler than those of $M(R)$ except that the first and the fourth of Eqs. (6.5) have to be combined. We shall give the results only for the matrices $A(\xi)$, $B(\xi)$, $C(\xi)$, and $E(\xi)$ which have more practical applications:

(1) $A^{(q)}(\xi)_{\nu\mu} \equiv M^{(q)}\left[\begin{pmatrix} 1 & \xi \\ 1 & -1 \end{pmatrix}\right]_{\nu\mu}$:

$$\begin{aligned}
A^{(q)}_{\nu\mu} &= A^{(q-1)}_{\nu\mu} + \xi A^{(q-1)}_{\nu,\mu-1} \\
&= A^{(q-1)}_{\nu-1,\mu} - A^{(q-1)}_{\nu-1,\mu-1}, \\
(q-\mu)A^{(q)}_{\nu\mu} &= (q-\nu)A^{(q-1)}_{\nu\mu} + \nu A^{(q-1)}_{\nu-1,\mu}, \\
\mu A^{(q)}_{\nu\mu} &= (q-\nu)\xi A^{(q-1)}_{\nu,\mu-1} - \nu A^{(q-1)}_{\nu-1,\mu-1}, \\
\frac{d}{d\xi} A^{(q)}_{\nu\mu} &= (q-\nu) A^{(q-1)}_{\nu,\mu-1}.
\end{aligned} \tag{6.9}$$

Using the first two recursion formulas one can show that the partial product defined by

$$\alpha^{(q,s)}_{\nu,\mu} = \sum_{\sigma=0}^{s} A^{(q)}_{\nu\sigma} A^{(q)}_{\sigma\mu}, \quad 0 \le s \le q, \tag{6.10}$$

satisfies the recursion formula

$$\alpha^{(q,s)}_{\nu\mu} = (1+\xi)\alpha^{(q-1,s-1)}_{\nu-1,\mu-1} + A^{(q)}_{\nu-1,s} A^{(q)}_{s,\mu}. \tag{6.11}$$

(2) $B(\xi)_{\nu\mu} = M\left[\begin{pmatrix} 1 & 0 \\ \xi & -1 \end{pmatrix}\right]_{\nu\mu} = \binom{\nu}{\mu} \xi^{\nu-\mu}(-1)^{\mu}$:

$$\begin{aligned}
B_{\nu\mu} &= \xi B_{\nu-1,\mu} - B_{\nu-1,\mu-1}, \\
(\nu-\mu)B_{\nu\mu} &= \xi\nu B_{\nu-1,\mu}, \\
\frac{d}{d\xi} B_{\nu\mu} &= \nu B_{\nu-1,\mu}.
\end{aligned} \tag{6.12}$$

From the first recursion formula one can show that, for $\nu \ge s \ge \mu$,

$$\sum_{\sigma=0}^{s} B_{\nu\sigma} B_{\sigma\mu} = (-1)^s \binom{\nu-\mu-1}{s-\mu} B_{\nu\mu}, \tag{6.13}$$

which has an important application in the transformation of spin–spin correlation functions of the Ising model.[1]

(3) $C(\xi)_{\nu\mu} = M^{(q)}\left[\begin{pmatrix} 1 & \xi \\ 0 & -1 \end{pmatrix}\right]_{\nu\mu} = \binom{q-\nu}{q-\mu} \xi^{\mu-\nu}(-1)^{\nu}$:

$$\begin{aligned}
C^{(q)}_{\nu\mu} &= C^{(q-1)}_{\nu\mu} + \xi C^{(q-1)}_{\nu,\mu-1} \\
&= -C^{(q-1)}_{\nu-1,\mu-1}, \\
\frac{d}{d\xi} C^{(q)}_{\nu\mu} &= (q-\nu) C^{(q-1)}_{\nu,\mu-1}.
\end{aligned} \tag{6.14}$$

(4) $E^{(q)}(\xi)_{\nu\mu} = M^{(q)}\left[\begin{pmatrix} \xi & 1 \\ 1 & -\xi \end{pmatrix}\right]_{\nu\mu}$:

$$\begin{aligned}
E^{(q)}_{\nu\mu} &= \xi E^{(q-1)}_{\nu\mu} + E^{(q-1)}_{\nu,\mu-1} \\
&= E^{(q-1)}_{\nu-1,\mu} - \xi E^{(q-1)}_{\nu-1,\mu-1}, \\
(q-\mu)E^{(q)}_{\nu\mu} &= (q-\nu)\xi E^{(q-1)}_{\nu\mu} + \nu E^{(q-1)}_{\nu-1,\mu-1}, \\
\mu E^{(q)}_{\nu\mu} &= (q-\nu)E^{(q-1)}_{\nu,\mu-1} - \xi\nu E^{(q-1)}_{\nu-1,\mu-1}, \\
\frac{d}{d\xi} E^{(q)}_{\nu\mu} &= (q-\nu)E^{(q-1)}_{\nu,\mu} - \nu E^{(q-1)}_{\nu-1,\mu-1}.
\end{aligned} \tag{6.15}$$

(5) Finally we shall give the recursion formula for the representation $S^{(q)}(R)$ which is defined by Eq. (5.7). The fundamental set of the recursion formulas of $M(R)$, Eqs. (6.3)–(6.5), gives the following for $S(R)$:

$$\begin{aligned}
(q-\nu)^{\frac{1}{2}} S^{(q)}_{\nu\mu} &= a(q-\mu)^{\frac{1}{2}} S^{(q-1)}_{\nu\mu} + b\mu^{\frac{1}{2}} S^{(q-1)}_{\nu,\mu-1}, \\
\nu^{\frac{1}{2}} S^{(q)}_{\nu\mu} &= c(q-\mu)^{\frac{1}{2}} S^{(q-1)}_{\nu-1,\mu} + d\mu^{\frac{1}{2}} S^{(q-1)}_{\nu-1,\mu-1}, \\
(q-\mu)^{\frac{1}{2}} S^{(q)}_{\nu\mu} &= a(q-\nu)^{\frac{1}{2}} S^{(q-1)}_{\nu,\mu} + c\nu^{\frac{1}{2}} S^{(q-1)}_{\nu-1,\mu}, \\
\mu^{\frac{1}{2}} S^{(q)}_{\nu\mu} &= b(q-\nu)^{\frac{1}{2}} S^{(q-1)}_{\nu,\mu-1} + d\nu^{\frac{1}{2}} S^{(q-1)}_{\nu-1,\mu-1},
\end{aligned} \tag{6.16}$$

$$\begin{aligned}
\frac{\partial}{\partial a} S^{(q)}_{\nu\mu} &= [(q-\nu)(q-\mu)]^{\frac{1}{2}} S^{(q-1)}_{\nu\mu}, \\
\frac{\partial}{\partial b} S^{(q)}_{\nu\mu} &= [(q-\nu)\mu]^{\frac{1}{2}} S^{(q-1)}_{\nu,\mu-1}, \\
\frac{\partial}{\partial c} S^{(q)}_{\nu\mu} &= [\nu(q-\mu)]^{\frac{1}{2}} S^{(q-1)}_{\nu-1,\mu}, \\
\frac{\partial}{\partial d} S^{(q)}_{\nu\mu} &= (\nu\mu)^{\frac{1}{2}} S^{(q-1)}_{\nu-1,\mu-1}.
\end{aligned} \tag{6.17}$$

Recursion formulas for this representation are rather cumbersome if not complicated. One could avoid this representation using $M(R)$ together with the symmetry property (5.6). If we use Eq. (5.17) we could write down all the recursion formulas for the Wigner function $\mathfrak{D}^j(U)$ as well.[4]

ACKNOWLEDGMENTS

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

Hyperplane Helicity States*

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(Received 7 February 1969)

The hyperplane formalism of Fleming is developed to include a discussion of the operations of the Poincaré group, as seen by an arbitrary hyperplane observer. Basis states for the $m > 0$ irreducible representations of the Poincaré group are re-expressed within the framework of generalized covariance provided by the hyperplane formalism and are seen to be related to the conventional helicity states by a special Lorentz transformation.

I. INTRODUCTION

Since the introduction of the helicity formalism by Jacob and Wick[1] in 1959, helicity states and amplitudes have become widely utilized in elementary particle physics. The helicity formalism has most fruitfully been applied in the theoretical development of and calculations involving dispersion relations,[2] resonance decay,[3] the absorption model,[4] and the Regge pole model.[5] Despite the elegance of the Jacob and Wick theory,[1] however, helicity amplitudes, although covariant in a true physical sense, are not "manifestly" so. This is, of course, related to the problems of kinematic singularities discussed by various authors.[6]

Fleming[7] has given a technique based on his "hyperplane" formalism for explicitly displaying the covariance of systems which are not manifestly covariant in the usual sense. One of the merits of Fleming's hyperplane formalism, as interpreted by Hammer, McDonald, and Pursey (HMP),[8] is that it provides a convenient, covariant way of describing various observers simultaneously with the observed physical system. Fleming[7] has shown that operators which are not usually considered to be covariant may be generalized to forms which, by relating to operators used by an arbitrary observer, are indeed manifestly covariant. This sense of manifest covariance is described in detail by HMP.[8]

The purpose of this paper is to construct helicity states within the framework of the hyperplane formalism. While the results are not expected to resolve any currently outstanding problems in the use of the helicity formalism, it is believed that further developments along these lines will lead to a considerably deeper insight into the relationship between the observed system and the observer.

The hyperplane formalism is, most simply, a restatement of the equivalence of the various inertial

* Work was performed in the Ames Laboratory of the U.S. Atomic Energy Commission. Contribution No. 2433.

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observers. In the Minkowski space, with signature $(+ - - -)$, spanned by a given orthogonal tetrad

$$\{e^\mu: \mu = 0, 1, 2, 3\} = \{(1, 0, 0, 0), (0, 1, 0, 0), (0, 0, 1, 0), (0, 0, 0, 1)\}, \tag{1}$$

an arbitrary spacelike hyperplane is defined by a unit normal η^μ, with $\eta_\mu \eta^\mu = 1$. The spacelike frame of every inertial observer may then be said to span a particular hyperplane. Fleming[7] has called the particular hyperplane with $\tilde{\eta}^\mu = (1, \mathbf{0})$ the "instantaneous" hyperplane and this hyperplane is spanned by the triad $\{e^i: i = 1, 2, 3\}$. The observer with this particular triad for a reference frame is called by HMP[8] the "superobserver." Observers associated with all other hyperplanes are accordingly called hyperplane observers.

Fleming[7] has constructed operators which generate infinitesimal transformations of the Poincaré group but which are not, in the usual sense, canonical. HMP[8] have shown how Fleming's operators may be constructed from the superobserver's canonical Poincaré generators by performing on them a Lorentz transformation which takes $\tilde{\eta}$ into the specified hyperplane normal η. In this paper, these operators will be shown to form what will be defined as a "supercanonical" set of infinitesimal Poincaré generators. It will be seen that this set of operators are those used by the superobserver to generate the Poincaré group as seen by a hyperplane observer. In Sec. III, the transformation parameters used by the superobserver are found explicitly in terms of the corresponding parameters used by the hyperplane observer. In Sec. IV, the helicity representation basis states for the $m > 0$ irreducible representations of the Poincaré group as seen by a hyperplane observer are constructed. In Sec. V, these hyperplane helicity states are related to the usual helicity states.

The HMP[8] interpretation of Fleming's operators[7] will be used, with the understanding that, unless otherwise specified, all transformations are to be taken in the "active" sense. That is, once the hyperplane observer's reference frame is defined, all Lorentz transformations will transform vectors and not reference frames. Also, as with Fleming,[7] the hyperplane normal η will always be a c-number so as to be identified with a macroscopic observer. As usual, units will be chosen such that $c = \hbar = 1$.

II. THE SUPERCANONICAL GENERATORS

The proper orthochronous Poincaré group is that group of transformations, with typical element (l, a), which carry the point with space–time coordinates x^μ into a point with coordinates x'^μ given by

$$x'^\mu = l^\mu_\nu x^\nu + a^\mu, \tag{2}$$

where

$$l^\mu_\nu l^\sigma_\mu = l^\sigma_\mu l^\mu_\nu = \delta^\sigma_\nu, \quad \det|l| = +1 \quad \text{and} \quad l^0_0 > 0. \tag{3}$$

Under the subgroup of homogeneous transformations of the form $(l, 0)$, the quantity $x_\mu x^\mu$ is left invariant. Here, the indices $\mu, \nu, \cdots$ label vector components with respect to the tetrad $\{e^\mu: \mu = 0, 1, 2, 3\}$ of Eq. (1).

The infinitesimal generators of $\mathfrak{P}$ are P^μ and $M^{\mu\nu}$, and satisfy the commutation rules

$$\begin{aligned} [P^\mu, P^\nu] &= 0, \\ [P^\mu, M^{\rho\sigma}] &= i(g^{\mu\rho}P^\sigma - g^{\mu\sigma}P^\rho), \\ [M^{\mu\nu}, M^{\rho\sigma}] &= i(g^{\mu\sigma}M^{\nu\rho} + g^{\nu\rho}M^{\mu\sigma} - g^{\mu\rho}M^{\nu\sigma} - g^{\nu\sigma}M^{\mu\rho}). \end{aligned} \tag{4}$$

No confusion will arise if the same symbols P^μ and $M^{\mu\nu}$ are used to denote both elements of the abstract Lie algebra of $\mathfrak{P}$ and the Hermitian operators which represent these generators in the state space of the quantum mechanical system under consideration. Corresponding to each $l \in \mathfrak{P}$, there is an operator L acting on the state space such that

$$\begin{aligned} L^{-1}P^\mu L &= l^\mu_\nu P^\nu, \\ L^{-1}M^{\mu\nu}L &= l^\mu_\delta l^\nu_\sigma M^{\delta\sigma}. \end{aligned} \tag{5}$$

In particular, the operator L is taken to be unitary and written as

$$L(\omega) = \exp \tfrac{1}{2} i\omega_{\mu\nu} M^{\mu\nu}, \tag{6}$$

where $\omega_{\mu\nu} = -\omega_{\nu\mu}$ so that, at most, only six of the components of ω are independent.

One may further define the operators

$$\begin{aligned} &J^i = \tfrac{1}{2}\epsilon^{ijk}M^{jk}, \quad N^i = M^{0i}, \quad i, j = 1, 2, 3, \\ &W^\mu = \tfrac{1}{2}\epsilon^{\mu\nu\delta\sigma}P_\nu M_{\delta\sigma}, \quad \text{with} \quad \epsilon^{1230} = \epsilon^{123} = +1. \end{aligned} \tag{7}$$

These operators satisfy the canonical commutation rules

$$\begin{aligned} &[P^\mu, P^\nu] = [P^\mu, W^\nu] = 0, \quad [P^0, J^i] = 0, \\ &[P^0, N^i] = iP^i, \quad [P^i, N^j] = i\delta^{ij}P^0, \\ &[J^i, J^j] = -[N^i, N^j] = i\epsilon^{ijk}J^k, \\ &[P^i, J^j] = i\epsilon^{ijk}P^k, \quad [J^i, N^j] = i\epsilon^{ijk}N^k. \end{aligned} \tag{8}$$

The P^μ generate four-translations, the J^i generate rotations, and the N^i generate "pure" Lorentz transformations, which are homogeneous transformations in the $i0$-planes. Moreover, the operators $P_\mu P^\mu$ and $W_\mu W^\mu$ are group invariants in that they commute with all of the group operations.

Since a homogeneous Lorentz transformation is, in general, specified by six parameters, three may be taken to be the parameters $\mathbf{u}$, say, of a pure Lorentz transformation l_0, and the remaining three the Euler angles α, β, γ for a rotation r. Thus, any such transformation $l(\omega)$ may be written as

$$l(\omega) = r(\alpha\beta\gamma)l_0(\mathbf{u}), \tag{9}$$

where the $\omega_{\mu\nu}$ may be found in terms of α, β, γ, and $\mathbf{u}$. The corresponding operator is given by

$$\begin{aligned} L[l(\omega)] &= R[r(\alpha\beta\gamma)]L_0[l_0(\mathbf{u})] \\ &= e^{i\alpha J^3}e^{i\beta J^2}e^{i\gamma J^3}e^{iu^1N^1}e^{iu^2N^2}e^{iu^3N^3}. \end{aligned} \tag{10}$$

Alternatively, the same transformation may be written as a Lorentz transformation $l(\eta)$ which takes the vector $\tilde{\eta} = (1, \mathbf{0})$ into the vector $\eta = ((1 + \boldsymbol{\eta}^2)^{\frac{1}{2}}, \boldsymbol{\eta})$, followed by a transformation $r(\eta; \omega')$ which leaves η fixed,

$$l(\omega) = r(\eta; \omega')l(\eta), \tag{11}$$

where $\eta^\mu = l^\mu_\nu(\eta)\tilde{\eta}^\nu$ and $r^\mu_\nu(\eta; \omega')\eta^\nu = \eta^\mu$. Following Fleming,[7] the vector η will henceforth be thought of as the unit normal to a hyperplane, the particular hyperplane with normal $\tilde{\eta}$ being called the "instantaneous" hyperplane. Each hyperplane will be associated with an observer who has velocity $\mathbf{v}$, say, relative to the superobserver. The transformation $l(\eta)$ of Eq. (11) is then given by

$$\begin{aligned} l^i_j(\eta) &= \delta^i_j - (\eta^i\eta_j)/(\eta^0 + 1), \\ l^i_0(\eta) &= l^0_i(\eta) = \eta^i, \quad l^0_0(\eta) = \eta^0 \geq 1, \end{aligned} \tag{12}$$

where the identifications $\eta^0 = (1 - \mathbf{v}^2)^{-\frac{1}{2}}$ and $\boldsymbol{\eta} = (1 - \mathbf{v}^2)^{-\frac{1}{2}}\mathbf{v}$ are made.

The transformation $l(\omega)$ of Eq. (11) will be completely defined only if a particular triad spanning the hyperplane, i.e., the hyperplane observer's spacelike frame, has been specified. For simplicity, a special hyperplane tetrad $\{\xi^{\mu'}: \mu = 0, 1, 2, 3\}$ will be defined in terms of the superobserver tetrad $\{e^\mu: \mu = 0, 1, 2, 3\}$ by

$$\begin{aligned} (\xi^{0'})^\mu &= l^\mu_\nu(\eta)(e^0)^\nu = l^\mu_0(\eta) = \eta^\mu, \\ (\xi^{i'})^\mu &= l^\mu_\nu(\eta)(e^i)^\nu = l^\mu_i(\eta). \end{aligned} \tag{13}$$

Here, the "primed" ("unprimed") subscripts and superscripts will label the hyperplane (superobserver) tetrad to which the subscript or superscript refers. As seen by the hyperplane observer, the tetrad of Eq. (13) is written as

$$\begin{aligned} &\{\xi^{\mu'}: \mu = 0, 1, 2, 3\} \\ &\quad = \{\xi^{0'}, \xi^{1'}, \xi^{2'}, \xi^{3'}\} \\ &\quad = \{[1, 0, 0, 0], [0, 1, 0, 0], [0, 0, 1, 0], [0, 0, 0, 1]\}, \end{aligned} \tag{14}$$

where the braces (brackets) enclose the components of a vector with respect to the hyperplane observer's (superobserver's) tetrad. For the instantaneous hyperplane, $l^\mu_\nu(\tilde{\eta}) = \delta^\mu_\nu$, so that the tetrad of Eq. (13) is the superobserver's tetrad, Eq. (1). From Eqs. (12) and (13), it is clear that

$$\begin{aligned} (\xi^{i'})^\mu\eta_\mu = (\xi^{i'})^\mu(\xi^{0'})_\mu &= 0, \\ (\xi^{i'})^\mu(\xi^{j'})_\mu &= \delta^{i'j'} = \delta^{ij}. \end{aligned} \tag{15}$$

Any other tetrad $\{\eta, \xi^{i''}: i = 1, 2, 3\}$ is then related to the special tetrad of Eq. (13) by a Lorentz transformation $r(\eta; \omega')$ so that specification of an arbitrary hyperplane observer's reference frame is equivalent to specification of η and $r(\eta; \omega')$. In the following discussion, the special tetrad of Eq. (13) will be taken to be the hyperplane observer's reference frame.

The transformations discussed from Eq. (9) to Eq. (15) are "passive" transformations, in the sense that reference frames are transformed. However, the "active" interpretation is desired in the following discussion. Hence, the hyperplane tetrads to be used henceforth will be taken to be known *a priori*, defined by relations of the type (7) and (13). Any other hyperplane tetrad may also be used, by specifying it *a priori* by Eq. (13), with $l(\eta)$ replaced by $r(\eta; \omega')l(\eta)$. With this understanding, there should be no ambiguity as to the interpretation of Lorentz transformations.

In order to discuss the Poincaré operations as used by a hyperplane observer, it is necessary to find the infinitesimal generators for these transformations. Following HMP,[8] one may use the transformation $l(\eta)$ of Eq. (12), with corresponding operator $L(\eta)$, to define the hyperplane operators

$$\begin{aligned} H(\eta) &= L(\eta)P^0L^{-1}(\eta), \\ K^\mu(\eta) &= l^\mu_i(\eta)L(\eta)P^iL^{-1}(\eta), \\ J^\mu(\eta) &= l^\mu_i(\eta)L(\eta)J^iL^{-1}(\eta), \\ N^\mu(\eta) &= l^\mu_i(\eta)L(\eta)N^iL^{-1}(\eta). \end{aligned} \tag{16}$$

By using Eqs. (3), (5), and (12), it follows that

$$\begin{aligned} H(\eta) &= \eta_\mu P^\mu, & K^\mu(\eta) &= P^\mu - \eta^\mu(\eta_\sigma P^\sigma), \\ J^\mu(\eta) &= \tfrac{1}{2}\epsilon^{\mu\rho\sigma\nu}M_{\rho\sigma}\eta_\nu, & N^\mu(\eta) &= M^{\mu\nu}\eta_\nu, \end{aligned} \tag{17}$$

which are the operators constructed by Fleming.[7] Furthermore, by using Eqs. (8) and (16), together with the identities

$$l^\mu_i(\eta)l^\nu_j(\eta)g^{ij} = g^{\mu\nu} - \eta^\mu\eta^\nu \tag{18}$$

and

$$l^\mu_i(\eta)l^\nu_j(\eta)L(\eta)\epsilon^{ijk}A^kL^{-1}(\eta) = -\epsilon^{\mu\nu\gamma\delta}A_\gamma(\eta)\eta_\delta, \tag{19}$$

where

$$A^\mu(\eta) = l^\mu_i(\eta)L(\eta)A^iL^{-1}(\eta) \tag{20}$$

with

$$A^k = P^k, J^k, \quad \text{and} \quad N^k,$$

one may show that

$$\begin{aligned}
&[K^\mu, K^\nu] = 0, \quad [H, J^\mu] = 0,\\
&[H, N^\mu] = iK^\mu, \quad [K^\mu, N^\nu] = -i(g^{\mu\nu} - \eta^\mu\eta^\nu)H,\\
&[J^\mu, J^\nu] = -[N^\mu, N^\nu] = -i\epsilon^{\mu\nu\rho\sigma}J_\rho\eta_\sigma,\\
&[K^\mu, J^\nu] = -i\epsilon^{\mu\nu\rho\sigma}K_\rho\eta_\sigma, \quad [J^\mu, N^\nu] = -i\epsilon^{\mu\nu\rho\sigma}N_\rho\eta_\sigma,
\end{aligned} \tag{21}$$

as was previously shown by Fleming.[7]

Since, from Eq. (17), the canonical generators P^μ, J^i, and N^i may be written as linear combinations of Fleming's operators,[7] then these operators also generate the Poincaré group. As seen by either the superobserver or a hyperplane observer, these operators are not canonical operators in the usual sense. The operators defined by Eq. (16) will henceforth be called "supercanonical" in that their commutation rules are the hyperplane generalization of the canonical rules of Eq. (8). In fact, Eq. (21), together with the constraints $(\eta K) = (\eta J) = (\eta N) = 0$, completely define the structure constants for the abstract Lie algebra of $\mathfrak{F}$. In the case of the instantaneous hyperplane $\tilde{\eta} = (1, \mathbf{0})$, the supercanonical generators are identical with the canonical generators P^μ, J^i, and N^i used by the superobserver.

The canonical generators used by a hyperplane observer may now be defined by

$$\begin{aligned}
P^{0'} &= H(\eta),\\
P^{i'} &= (\xi^{i'})_\mu K^\mu(\eta) = l^i_\mu(\eta)K^\mu(\eta),\\
J^{i'} &= (\xi^{i'})_\mu J^\mu(\eta) = l^i_\mu(\eta)J^\mu(\eta),\\
N^{i'} &= (\xi^{i'})_\mu N^\mu(\eta) = l^i_\mu(\eta)N^\mu(\eta).
\end{aligned} \tag{22}$$

It follows that, by using Eqs. (16) and (22),

$$\mathcal{O}^{\alpha'} = L(\eta)\mathcal{O}^\alpha L^{-1}(\eta) \tag{23}$$

where $\mathcal{O}^{\alpha'}(\mathcal{O}^\alpha)$ is one of the canonical generators $P^{\alpha'}, J^{\alpha'}, N^{\alpha'}(P^\alpha, J^\alpha, N^\alpha)$ used by the hyperplane observer (superobserver). Conversely, the supercanonical generators may be written in terms of the hyperplane observer's canonical generators

$$\begin{aligned}
H &= P^{0'},\\
K^\mu &= l^\mu_i P^{i'},\\
J^\mu &= l^\mu_i J^{i'},\\
N^\mu &= l^\mu_i N^{i'}.
\end{aligned} \tag{24}$$

By defining the quantities

$$\begin{aligned}
g_{i'j'} &= (\xi_{i'})^\mu(\xi_{j'})^\nu(g_{\mu\nu} - \eta_\mu\eta_\nu),\\
\epsilon_{i'j'k'} &= (\xi_{i'})^\mu(\xi_{j'})^\nu(\xi_{k'})^\rho(\xi_{0'})^\sigma\epsilon_{\mu\nu\rho\sigma},
\end{aligned} \tag{25}$$

one may show that $P^{\alpha'}$, $J^{\alpha'}$, $N^{\alpha'}$ satisfy Eq. (6), with primes on all indices. Hence, the operators of Eq. (22) are indeed the canonical Poincaré generators used by the hyperplane observer whose reference frame is the tetrad of Eq. (13).

An operator which will be seen in Sec. IV to be of considerable interest is the helicity operator Π. For the $m > 0$ irreducible representations, the helicity operator used by the superobserver is given by

$$\Pi = J_i P_i (P_j P_j)^{-\frac{1}{2}}. \tag{26}$$

Correspondingly, the hyperplane observer used the operator

$$\Pi(\eta) = J_{i'}P_{i'}(P_{j'}P_{j'})^{-\frac{1}{2}} \tag{27}$$

for his helicity. In terms of the supercanonical generators, this hyperplane helicity operator is, from Eq. (22),

$$\Pi(\eta) = -J_\mu K^\mu(-K_\nu K^\nu)^{-\frac{1}{2}} \tag{28}$$

which, for the instantaneous hyperplane, is just Π of Eq. (26).

III. HYPERPLANE TRANSFORMATIONS

From Eqs. (17) and (24), it should be clear that the supercanonical operators H, K^μ, J^μ, and N^μ generate $\mathfrak{F}$ as seen by either the superobserver or a hyperplane observer. H and K^μ generate translations normal to and parallel to the hyperplane, respectively, and the J^μ generate homogeneous transformations within the hyperplane. Transformations generated by the J^μ will be called "hyperplane rotations" since the J^μ generate a group isomorphic with the group of three-dimensional rotations. Furthermore, the N^μ generate homogeneous transformations in all planes containing η, transformations which a hyperplane observer sees as pure Lorentz transformations. From Eqs. (17) and (12), it is easy to see the relationships between the various transformation parameters used by the hyperplane observer and those used by the superobserver.

For an arbitrary translation $t(a)$, the hyperplane observer uses the operator

$$T(\eta; t(a)) = e^{-ia_{\mu'}P^{\mu'}} = e^{i(\alpha_\mu K^\mu - \tau H)}, \tag{29}$$

where $\alpha_\mu = l^i_\mu(\eta)\, a^{i'}$ and $\tau = a^{0'}$. For the same translation, the superobserver then uses the operator

$$T[t(a)] = e^{-ia_\mu(\eta)P^\mu} = e^{i(\alpha_\mu K^\mu - \tau H)}, \tag{30}$$

where it follows that

$$a^\mu(\eta) = l^\mu_\nu(\eta)a^{\nu'}. \tag{31}$$

An arbitrary hyperplane rotation $r(\eta)$ may be parametrized in terms of the Euler angles α, β, γ as seen by the hyperplane observer, with corresponding operator

$$\begin{aligned}
R[\eta; r(\eta; \alpha\beta\gamma)] &= e^{i\alpha J^{3'}}e^{i\beta J^{2'}}e^{i\gamma J^{3'}}\\
&= e^{i\alpha_\mu(\eta,\alpha)J^\mu}e^{i\beta_\mu(\eta,\beta)J^\mu}e^{i\gamma_\mu(\eta,\gamma)J^\mu},
\end{aligned} \tag{32}$$

where

$$\alpha_\mu = \alpha l^3_\mu(\eta), \quad \beta_\mu = \beta l^2_\mu(\eta), \quad \text{and} \quad \gamma_\mu = \gamma l^3_\mu(\eta).$$

The superobserver's operator is

$$L[\omega(\eta; r(\alpha\beta\gamma))] = e^{i\frac{1}{2}\omega_{\mu\nu}((3',\alpha)M^{\mu\nu}} e^{i\frac{1}{2}\omega_{\mu\nu}(2',\beta)M^{\mu\nu}} e^{i\frac{1}{2}\omega_{\mu\nu}(3',\gamma)M^{\mu\nu}}, \quad (33)$$

where

$$\begin{aligned}\omega_{\mu\nu}(3', \alpha) &= \alpha\epsilon_{\mu\nu\rho\sigma} l^\rho_3(\eta)\eta^\sigma,\\ \omega_{\mu\nu}(2', \beta) &= \beta\epsilon_{\mu\nu\rho\sigma} l^\rho_2(\eta)\eta^\sigma.\end{aligned} \quad (34)$$

Similarly, a pure Lorentz transformation as seen by the hyperplane observer has the operator

$$L[\eta; \omega(u)] = e^{iu^{i'}N^{i'}} = e^{iv_\mu(u_{i'})N^\mu}, \quad (35)$$

with $v_\mu(u_{i'}) = l^i_\mu(\eta)u^{i'}$. As seen by the superobserver,

$$L[\omega(\eta; u)] = e^{i\frac{1}{2}\omega_{\mu\nu}(\eta;u)M^{\mu\nu}}, \quad (36)$$

where

$$\omega_{\mu\nu}(\eta, u) = v_\mu\eta_\nu - v_\nu\eta_\mu = (l^i_\mu\eta_\nu - l^i_\nu\eta_\mu)u^{i'}. \quad (37)$$

IV. HYPERPLANE HELICITY STATES

The basis states for the irreducible representations of $\mathfrak{I}$, as seen by a hyperplane observer, may now be constructed. Here, only the $m > 0$ case will be considered. As in the conventional treatment,[1] basis states are labeled by the eigenvalues of the various hyperplane observer's operators, consistent with Eq. (8) with primes on all indices: $|\eta; (ms)\epsilon p\lambda\rangle$, which satisfies

$$\begin{aligned}P^{i'}|\eta; (ms)\epsilon p\lambda\rangle &= p^{i'}|\eta; (ms)\epsilon p\lambda\rangle,\\ p^{0'}|\eta; (ms)\epsilon p\lambda\rangle &= \epsilon(p_{j'}p_{i'} + m^2)^{\frac{1}{2}}|\eta; (ms)\epsilon p\lambda\rangle,\\ \hat{\epsilon}(\eta)|\eta; (ms)\epsilon p\lambda\rangle &= \epsilon|\eta; (ms)\epsilon p\lambda\rangle,\\ \Pi(\eta)|\eta; (ms)\epsilon p\lambda\rangle &= \lambda|\eta; (ms)\epsilon p\lambda\rangle,\end{aligned} \quad (38)$$

where $\hat{\epsilon}(\eta) = P^{0'}/|P^{0'}|$ is the hyperplane observer's sign-of-the-energy operator and $\Pi(\eta)$ is his helicity operator, given by Eq. (27). Here, p is taken to represent $[p^{1'}, p^{2'}, p^{3'}]$. The first entry in the ket symbol, followed by a semicolon, is used to specify the observer's tetrad. In this case, η specifies the special hyperplane tetrad of Eq. (13).

The normalization is taken to be

$$\langle\eta; (ms')\epsilon'p'\lambda' \mid \eta; (ms)\epsilon p\lambda\rangle = 2\omega(p)\delta_{s's}\delta_{\epsilon'\epsilon}\delta_{\lambda'\lambda}\delta^3(p' - p), \quad (39)$$

where $\omega(p) = (p_{i'}p_{i'} + m^2)^{\frac{1}{2}}$. These states are, as seen by the hyperplane observer, the same as the conventional states used by the superobserver.

Using the little-group technique,[9] one defines the state $|\eta; (ms)\epsilon 0\lambda\rangle$ which corresponds to a hyperplane standard four-momentum $\tilde{p} = \epsilon m[1, 0, 0, 0]$, such that

$$P^{\mu'}|\eta; (ms)\epsilon 0\lambda\rangle = \tilde{p}^{\mu'}|\eta; (ms)\epsilon 0\lambda\rangle. \quad (40)$$

As seen by the superobserver, this standard momentum is $\tilde{p}^\mu = \epsilon m\eta^\mu$. The parameter λ is defined to be the component of spin in the $\xi^{3'}$ direction so that

$$J^{3'}|\eta; (ms)\epsilon 0\lambda\rangle = \lambda|\eta; (ms)\epsilon 0\lambda\rangle. \quad (41)$$

The little group is the group of transformations which leave $\tilde{p}$ fixed, which is in this case the group of hyperplane rotations, $\mathcal{R}(\eta)$. Under operations of $\mathcal{R}(\eta)$, the states of Eq. (40) transform according to

$$R(\eta, r(\eta; \alpha\beta\gamma))|\eta; (ms)\epsilon 0\lambda\rangle = \sum_\mu \mathfrak{D}^s_{\mu\lambda}[r(\eta; \alpha\beta\gamma)]|\eta; (ms)\epsilon 0\mu\rangle, \quad (42)$$

where $r(\eta; \alpha\beta\gamma)$ is a hyperplane rotation with Euler angles α, β, γ, and with corresponding operator $R[\eta; r(\eta; \alpha\beta\gamma)]$ given by Eq. (32). Also, $\mathfrak{D}^s(r)$ is the usual $(2s + 1)$-dimensional irreducible representation matrix of the rotation group.

The general state is then defined by

$$|\eta; (ms)\epsilon p\lambda\rangle = H^\epsilon_0(\eta; p)|\eta; (ms)\epsilon 0\lambda\rangle, \quad (43)$$

where

$$H^\epsilon_0(\eta; p) = R(\eta; r(\mathbf{p}))Z^\epsilon(\eta; z^\epsilon(\mathbf{p}')). \quad (44)$$

The transformation $z^\epsilon(\eta; \mathbf{p}')$, with operator $Z^\epsilon(\eta; z'(\mathbf{p}'))$, is a Lorentz transformation in the $\xi^{3'}$ direction such that

$$z^\epsilon(\eta; \mathbf{p}')\tilde{p} = p' = [\epsilon(m^2 + p^2)^{\frac{1}{2}}, 0, 0, p], \quad (45)$$

with $p = (p_{i'}p_{i'})^{\frac{1}{2}}$. The transformation $r(\mathbf{p})$, with operator $R(\eta; r(\mathbf{p}))$, is a hyperplane rotation such that

$$r(\mathbf{p})p' = p = [\epsilon(m^2 + p^2)^{\frac{1}{2}}, p^{1'}, p^{2'}, p^{3'}]. \quad (46)$$

The general state defined by Eq. (43) is then seen to transform under a general hyperplane transformation $l(\eta, \omega(\eta))$ according to

$$L[\eta; l(\eta; \omega)]|\eta; (ms)\epsilon p\lambda\rangle = \sum_\mu \mathfrak{D}^s_{\mu\lambda}[t(\eta; l)]|\eta; (ms)\epsilon p'\mu\rangle, \quad (47)$$

where

$$p'_{j'} = l^{i'}_{j'}(\eta; \omega(\eta))p_{i'} \quad (48)$$

and

$$t[\eta; l] = h^\epsilon_0(\eta; l\tilde{p})^{-1}lh^\epsilon_0(\eta, \tilde{p})$$

is an element of the little group $\mathcal{R}(\eta)$, with operator

$$T[\eta; l(\eta, \omega)] = H^\epsilon_0[\eta, l\tilde{p}]^{-1}L(\eta; l)H^\epsilon_0(\eta, \tilde{p}). \quad (49)$$

From Eqs. (41), (43), (27), and

$$H_0^{-1}\Pi(\eta)H_0 = Z'^{-1}\Pi(\eta)Z' = J^{3'}, \quad (50)$$

it follows that

$$\Pi(\eta)|\eta; (ms)\epsilon p\lambda\rangle = \lambda|\eta; (ms)\epsilon p\lambda\rangle. \quad (51)$$

[9] L. P. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. **50**, 58 (1936); E. P. Wigner, Ann. Math. **40**, 149 (1939).

Hence, the general hyperplane state of Eq. (43) is an eigenstate of the hyperplane helicity operator $\Pi(\eta)$, λ being interpreted as the component of spin in the direction of $p = [p^{1'}, p^{2'}, p^{3'}]$. For the particular case of the instantaneous hyperplane, these states are identical with the conventional helicity states:

$$|\tilde{\eta};(ms)\epsilon p\lambda\rangle = |(ms)\epsilon p\lambda\rangle. \tag{52}$$

It was seen in Sec. III that the Poincaré group as seen by a hyperplane observer may also be parametrized in terms of superobserver variables. Indeed, by utilizing the intermediate status of the supercanonical generators, the hyperplane helicity states may now be written in terms of parameters used by the superobserver. Such states may be defined by

$$|\tilde{\eta};(ms),\epsilon(\eta),k(\eta),\lambda(\eta)\rangle = |\eta;(ms)\epsilon p\lambda\rangle, \tag{53}$$

where $k_\mu = (\xi^{i'})_\mu p_{i'} = l^i_\mu(\eta)p_{i'}$ is the hyperplane momentum as seen by the superobserver. Where the context permits, these states will be written as $|\tilde{\eta};(ms)\epsilon k\lambda\rangle$, where it is understood that $k = k(\eta)$, $\epsilon = \epsilon(\eta)$, and $\lambda = \lambda(\eta)$. Due to the constraint $\eta_\mu k^\mu = 0$, the symbol $k(\mu)$ in the ket of Eq. (53) need only represent (k^1, k^2, k^3). Then, from Eqs. (24) and (38), it follows that

$$\begin{aligned} H(\eta)\,|\tilde{\eta};(ms)\epsilon k\lambda\rangle &= \epsilon(m^2 + k^2)^{\frac{1}{2}}\,|\tilde{\eta};(ms)\epsilon k\lambda\rangle,\\ K^\mu(\eta)\,|\tilde{\eta};(ms)\epsilon k\lambda\rangle &= k^\mu\,|\tilde{\eta};(ms)\epsilon k\lambda\rangle,\\ \hat{\epsilon}(\eta)\,|\tilde{\eta};(ms)\epsilon k\lambda\rangle &= \epsilon\,|\tilde{\eta};(ms)\epsilon k\lambda\rangle,\\ \Pi(\eta)\,|\tilde{\eta};(ms)\epsilon k\lambda\rangle &= \lambda\,|\tilde{\eta};(ms)\epsilon k\lambda\rangle, \end{aligned} \tag{54}$$

where $k^2 = -k_\mu k^\mu \geq 0$ and $k^0 = \boldsymbol{\eta}\cdot\mathbf{K}/\eta^0$ is well defined. From Eq. (47), these states are seen to transform according to

$$L[l(\eta,\omega)]\,|\tilde{\eta};(ms)\epsilon k\lambda\rangle = \sum_\mu \mathfrak{D}^s_{\mu\lambda}[t(\eta,l)]\,|\tilde{\eta};(ms)\epsilon k^1\mu\rangle, \tag{55}$$

where $k'_\mu = l^\nu_\mu(\eta, l(\eta,\omega))k_\nu$ with

$$\begin{aligned} l^\nu_\mu(\eta;l(\eta;\omega)) &= l^i_\mu(\eta)l^{j'}_{i'}(\eta;\omega)l^\nu_j(\eta)\\ &= (\xi^{i'})_\mu l^{j'}_{i'}(\eta;\omega)(\xi_{j'})^\nu. \end{aligned} \tag{56}$$

By using Eqs. (33) and (36), the hyperplane observer's operators $L(\eta, l)$ and $T(\eta, t)$ have been replaced by the corresponding operators $L(l(\eta,\omega))$ and $T(i(\eta;\omega))$ used by the superobserver.

The normalization of the hyperplane states of Eq. (53) is found by considering the invariant integral

$$I = \int \frac{d^3p}{2\omega(p)}\,\langle\eta;(ms')\epsilon'p'\lambda'\,|\,\eta;(ms)\epsilon p\lambda\rangle = \delta_{s's}\delta_{\epsilon'\epsilon}\delta_{\lambda'\lambda} \tag{57}$$

used by the hyperplane observer. This integration can be extended to $p^{0'}$ by noting that since $d^3p = dp^{1'}\,dp^{2'}\,dp^{3'}$ and

$$\int d^3pF(p) = \int d^3pF(p)\int dp^{0'}\delta(p^{0'}) = \int d^4pF(p)\delta(p^{0'}), \tag{58}$$

then

$$I = \int \frac{d^4p}{2\omega(p)}\,\delta(p^{0'})\langle\eta;(ms')\epsilon'p'\lambda'\,|\,\eta;(ms)\epsilon p\lambda\rangle. \tag{59}$$

Alternatively, the variable transformation $p_{\mu'} = l^\nu_\mu(\eta)k_\nu$ yields

$$I = \int \frac{d^4k\delta(\eta k)}{2(m^2+k^2)^{\frac{1}{2}}}\,\langle\tilde{\eta};(ms')\epsilon'k'\lambda'\,|\,\tilde{\eta};(ms)\epsilon k\lambda\rangle, \tag{60}$$

where $k^2 = -k_\mu k^\mu$, and $d^4p = d^4k$ and $p^{0'} = l^\nu_0 k_\nu = \eta^\nu k_\nu$ have been used. Hence, the normalization is given by

$$\langle\tilde{\eta};(ms')\epsilon'k'\lambda'\,|\,\tilde{\eta};(ms)\epsilon k\lambda\rangle = \delta_{s's}\delta_{\epsilon'\epsilon}\delta_{\lambda'\lambda}\tilde{\delta}(k'-k), \tag{61}$$

where, analogous to the usual Lorentz invariant $\tilde{\delta}(p'-p) = 2\omega(p)\delta^3(p'-p)$,

$$\tilde{\delta}(k'-k) \equiv 2\eta^0\left[m^2 + k_ik_i - \left(\frac{\eta_ik_i}{\eta^0}\right)^2\right]^{\frac{1}{2}}\delta^3(k'-k). \tag{62}$$

V. CONNECTION BETWEEN HYPERPLANE STATES AND CONVENTIONAL HELICITY STATES

To see the connection between the Poincaré basis states of the hyperplane observer and the conventional helicity states used by the superobserver, it is perhaps easiest to first note that the hyperplane rest states of Eq. (40) are related to the conventional rest states[1] by the transformation $l(\eta)$ of Eq. (12):

$$|\eta;(ms)\epsilon 0\lambda\rangle = L(\eta)\,|\tilde{\eta};(ms)\epsilon 0\lambda\rangle, \tag{63}$$

where

$$l(\eta)(\epsilon m,\mathbf{0}) = \epsilon m l(\eta)\tilde{\eta} = \epsilon m\eta = [\epsilon m,\mathbf{0}]. \tag{64}$$

The transformation $l(\eta)$ may be used either in the passive sense, in which case it transforms the tetrad $\{e^\mu\}$ into $\{\xi^{\mu'}\}$, as seen by $l(\eta)$ $(\epsilon m,\mathbf{0}) = [\epsilon m,\mathbf{0}]$, or in the active sense, in which case it transforms $p_0 = (\epsilon m,\mathbf{0})$ into $\tilde{p}^\mu = \epsilon m\eta^\mu$. Acting on the ket vector used by the superobserver, $L(\eta)$ must be taken in the active sense, since the ket is associated with the fixed superobserver tetrad $\{e^\mu\}$. Appearance of the passive possibility is due to the definition, Eq. (13), of the hyperplane observer's tetrad.

Using the transformation property Eq. (55) for the instantaneous hyperplane states, which have been

seen to be identical with the conventional states,[1] Eq. (63) becomes

$$|\eta; (ms)\epsilon 0\lambda\rangle = \sum_{\mu} \mathfrak{D}^{s}_{\mu\lambda}[t(\tilde{\eta}; l(\eta))]\, |\tilde{\eta}; (ms)\epsilon\tilde{p}\mu\rangle, \quad (65)$$

where $\tilde{p}^{\mu} = \epsilon m \eta^{\mu}$ and

$$t(\tilde{\eta}; l(\eta)) = H_0^{\epsilon}(\tilde{\eta}; l(\eta)\tilde{p})^{-1} L(\eta) H_0^{\epsilon}(\tilde{\eta}; \tilde{p}) \quad (66)$$

is an element of the group of rotations in the instantaneous hyperplane. Also, from Eq. (23), it follows that $J^{3'} = L(\eta)J^3L^{-1}(\eta)$ so that the helicity interpretation is clearly preserved:

$$\begin{aligned} J^3\, |\tilde{\eta}; (ms)\epsilon 0\lambda\rangle &= L^{-1}(\eta)J^{3'}L(\eta)L^{-1}(\eta)\, |\eta; (ms)\epsilon 0\lambda\rangle \\ &= \lambda\, |\tilde{\eta}; (ms)\epsilon 0\lambda\rangle. \end{aligned} \quad (67)$$

From Eq. (43), the general state for the instantaneous hyperplane is given by

$$|\tilde{\eta}; (ms)\epsilon p\lambda\rangle = H_0^{\epsilon}(\tilde{\eta}; \mathbf{p})\, |\tilde{\eta}; (ms)\epsilon 0\lambda\rangle, \quad (68)$$

with

$$p = h_0^{\epsilon}(\mathbf{p})p_0 = r(\mathbf{p})z_0^{\epsilon}(\mathbf{p})p_0. \quad (69)$$

Here, $h_0^{\epsilon}(\mathbf{p}) \equiv h_0^{\epsilon}(\tilde{\eta}, \mathbf{p})$ is a Lorentz transformation $z_0^{\epsilon}(\mathbf{p})$ in the e^3 direction which takes $p_0 = (\epsilon m, \mathbf{0})$ into $p' = (\epsilon(m^2 + p^2)^{\frac{1}{2}}, 0, 0, p)$, followed by a rotation $r(\mathbf{p}) = r(\tilde{\eta}, \mathbf{p})$ which takes p' into $p = (\epsilon(m^2 + p^2)^{\frac{1}{2}}, \mathbf{p})$. Then, by using Eqs. (43), (63), and (66), the connection is found to be

$$|\eta; (ms)\epsilon p'\lambda\rangle = H_0^{\epsilon}(\eta; p)L(\eta)H_0^{\epsilon^{-1}}(\tilde{\eta}, p)\, |\tilde{\eta}; (ms)\epsilon p\lambda\rangle, \quad (70)$$

with

$$p' = h_0^{\epsilon}(\eta; \mathbf{p}')l(\eta)h_0^{\epsilon}(\tilde{\eta}; \mathbf{p})^{-1}p, \quad (71)$$

and p' and p refer to the same momentum vector as seen by the hyperplane observer and superobserver, respectively. However, from Eqs. (12) and (13), one also sees that

$$p'_{\mu'} = (\xi_{\mu'})^{\nu}p_{\nu} = l^{\nu}_{\mu}(\eta)p_{\nu} = (l^{-1}(\eta)p)_{\mu}. \quad (72)$$

This comes about owing to the definition of the hyperplane tetrad $\{\xi^{\mu'}\}$ so that, in Eq. (72), the transformation $l(\eta)$ must be interpreted in the passive sense. With the understanding that the corresponding active and passive transformation operators are related by $L_{\text{act}} = L^{-1}_{\text{pass}}$, it follows that

$$H_0^{\epsilon}(\eta; \mathbf{p}')L(\eta)H_0^{\epsilon}(\tilde{\eta}; \mathbf{p})^{-1} = L(\eta) \quad (73)$$

with the active interpretation. Hence, Eq. (70) simplifies to

$$|\tilde{\eta}; (ms)\epsilon p'\lambda\rangle = L(\eta)\, |\tilde{\eta}; (ms)\epsilon p\lambda\rangle. \quad (74)$$

The superobserver's hyperplane helicity state is then related to his helicity state by

$$|\tilde{\eta}; (ms), \epsilon(\eta), k(\eta), \lambda(\eta)\rangle = L(\eta)\, |\tilde{\eta}; (ms)\epsilon p\lambda\rangle, \quad (75)$$

with

$$k_{\mu}(\eta) = l^{i}_{\mu}(\eta)p'_{i'} = l^{i}_{\mu}(\eta)l^{\nu}_{i}(\eta)p_{\nu} = p_{\mu} - \eta_{\mu}(\eta^{\nu}p_{\nu}).$$

It then follows that the connection between the states used by observers on two different hyperplanes η_1 and η_2, with corresponding tetrads $\{\xi'_{\mu_1}\}$ and $\{\xi_{\mu_2}\}$ defined by Eq. (13), is given by

$$|\eta_2; (ms)\epsilon p_2\lambda\rangle = L(\eta_2)L^{-1}(\eta_1)\, |\eta_1; (ms)\epsilon p_1\lambda\rangle \quad (76)$$

where $(p_2)_{\mu'} = l^{\nu}_{\mu}(\eta_2)l^{\sigma}_{\nu}(\eta_1)(p_1)_{\sigma'}$. The superobserver's hyperplane helicity states for the two hyperplanes are then related by

$$\begin{aligned} &|\tilde{\eta}; (ms), \epsilon(\eta_2), k(\eta_2), \lambda(\eta_2)\rangle \\ &\quad = L(\eta_2)L^{-1}(\eta_1)\, |\tilde{\eta}; (ms), \epsilon(\eta_1), k(\eta_1), \lambda(\eta_1)\rangle, \end{aligned} \quad (77)$$

where

$$\begin{aligned} k_i(\eta_2) &= (\delta^{\nu}_i - \eta_{2i}\eta_2^{\nu})[k_{\nu}(\eta_1) + h_1\eta_{1\nu}], \\ h_1 &= (p_1)_{0'} = \epsilon(m^2 - k_{1\mu}k_1^{\mu})^{\frac{1}{2}}, \\ k_{\mu}(\eta_1)\eta_1^{\mu} &= k_{\mu}(\eta_2)\eta_2^{\mu} = 0. \end{aligned} \quad (78)$$

ACKNOWLEDGMENT

The author would like to thank Professor D. L. Pursey for many valuable discussions.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

S-Matrix and Classical Description of Interactions*

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(Received 29 November 1966)

It is shown quite generally, through a correspondence between S-matrix and classical descriptions of particle states and of their measurements, that an S-matrix theory actually leads, under appropriate conditions, to the classical space-time description of interactions, involving the usual classical concepts and formulas.

I. INTRODUCTION

Does S-matrix theory describe such complicated processes as the creation of straight tracks in a bubble chamber? This is the kind of questions that we aim to solve.

The above process is usually described in a classical way. In that classical description, since particles propagate in space-time, they can be submitted to some measurement or can have some interaction with other particles. The concepts of localization in space-time, of locality of an interaction, of causality, and of separate or successive interactions are used and corresponding formulas are written.

On the other hand, the theorist introduces an S-matrix formalism to which all the above concepts are foreign at first.

Our purpose is not only to study which more or less qualitative hints indicate that S-matrix theory could actually describe the processes quoted above, but mainly to show, through a correspondence between S-matrix and classical descriptions, that, under special conditions, S-matrix theory actually leads to the usual classical description and formulas.

What we are going to do is, then, as follows.

In Sec. II, we recall the general features of S-matrix formalism and study to what extent some general properties of the S matrix can be good candidates to account for classical concepts.

In Sec. III, we establish a correspondence between S-matrix and classical descriptions of particle states and their measurement apparatus and study why, when, and to what extent it is a good candidate in order to compare S-matrix and classical results.

In Sec. IV (for single scattering) and Sec. V (for multiple scattering), we will then actually show how S-matrix theory leads to the classical formulas for transition probabilities in many interesting cases.

In Sec. VI, we show how these results lead to the usual classical description of preparation and evolution of a state and as an example, we answer the above straight-tracks problem.

Spinless particles with nonzero masses are considered and we adopt a system with $\hbar = c = 1$.

II. S-MATRIX FORMALISM: GENERAL PROPERTIES

The general features of an S-matrix formalism are given in Sec. II.A. Sections II.B–II.D are devoted to the study of the general properties which can account for the classical concepts and formulas.

Among those, some are closely related to the classical aspect of the description of the states (localization in space-time, locality of an interaction, etc.). Some others can be stated in the form of a property (P) of the transition probability, which is independent of the detailed description of the states, involving only space-time translations of states.

This concept of space-time translations is introduced in S-matrix formalism by assuming the existence of a representation of the Poincaré group in the Hilbert space of states; a usual line of thought is the following: the property (P) of the transition probability will also be assumed, in some way to be made precise, in S-matrix theory. One looks for the induced property of the S matrix or S-matrix elements, which we call (H).

Conversely, one determines if some hypothesis of type (H) gives back property (P)—at least under special conditions. If these are less restrictive than the conditions used to obtain the classical formulas, it is reasonable to think that the hypothesis (H) actually accounts for the classical concept and formula corresponding to (P).

In Sec. II.B, we study how Poincaré invariance of the transition probability is related to the "energy-momentum conservation" of the S matrix. In Sec. II.C, we study how some cluster property of the transition probability is related with a property of the connected

* This work is an enlarged and revised version of "S-Matrix Theory and Phenomenological Space-Time Description," University of California, Berkeley, preprint.

amplitudes of a cluster decomposition (following Refs. 1 and 2).

It is tempting to use this approach in order to account for the classical concept of successive (or multiple) scatterings. However, it becomes in that case rather ad hoc to get precise results. A general discussion is given in Sec. II.D and a more precise short account of what can be said is given in Appendix A.

A. General Features

The S matrix is usually understood as an isometry of a Hilbert space $\mathcal{H}$.

In the following, we consider the usual Fock space. One-particle states are the space $L^2(R^3)$ of square-integrable functions and many-particles states are described in the corresponding Fock representation.

The transition operator T is defined through

$$S = 1 + iT. \tag{1}$$

An ensemble of final states of n particles is described by an efficiency matrix F_n. The operator F_n is Hermitian and positive-definite, as is $1_n - F_n$ as well, where 1_n is the identity operator of the subspace of n-particle states and

$$0 \leq F_n \leq 1_n. \tag{2}$$

With some orthonormal basis $|\varphi_i\rangle$, F can be written as $F = \sum_i c_i |\varphi_i\rangle\langle\varphi_i|$, where the efficiency coefficients c_i for the state $|\varphi_i\rangle$ are positive and less than unity. It leads to the general characterization given here in Eq. (2).

As is well known, a density matrix, furthermore, satisfies the equation $\sum_i c_i = 1$ which leads to Eq. (3).

An initial state of m particles is similarly described by a density matrix ζ_m which satisfies

$$0 \leq \zeta_m \leq 1 \tag{2'}$$

and, furthermore,

$$\mathrm{Tr}_{(m)}\, \zeta_m = 1. \tag{3}$$

The transition probability W of an initial state described by the density matrix ζ_m, when the measurement apparatus is described through the efficiency matrix F_n, is

$$W = \mathrm{Tr}\, \zeta_m T_{mn} F_n T^{\dagger}_{mn}, \tag{4}$$

where T_{mn} is the restriction of T to the initial space of m particles and the final space of n particles.

Because of the above properties of ζ, F, and T, the transition probability W enjoys the expected property

$$0 \leq W \leq 1. \tag{5}$$

In the following, it will be useful to consider the kernels associated with the operators T_{mn}, S_{mn}, ζ_m, F_n in the momentum representation.

The normalization will be

$$\begin{gathered} \int \frac{d\mathbf{p}}{2p_0} |\mathbf{p}\rangle\langle\mathbf{p}| = 1, \\ \langle \mathbf{p} \mid \mathbf{p}' \rangle = 2p_0 \delta(\mathbf{p} - \mathbf{p}'), \\ p_0 = (\mathbf{p}^2 + m^2)^{\frac{1}{2}}. \end{gathered} \tag{6}$$

The kernels exist as temperate distributions, the order of which can be bounded. Consider, for the sake of simplicity, an operator A bounded from $L^2(R^3)$ to $L^2(R^3)$. It can be extended to a continuous operator from $\mathcal{S}$ to $\mathcal{S}'$, which implies that the kernel exists as a temperate distribution due to the nuclear theorem. As it is, furthermore, continuous from $L^2(R^2)$ to $L^2(R^3)$, the order of this distribution can be shown to be bounded by Eq. (4). Due to properties (2'), (3), the kernel $\zeta_m(\mathbf{p}_1 \cdots \mathbf{p}_m, \mathbf{p}'_1 \cdots \mathbf{p}'_m)$ is also a square-integrable function

$$\int |\zeta_m(\mathbf{p}_1 \cdots, \mathbf{p}'_1 \cdots)|^2 \frac{d\mathbf{p}_1}{2p_{10}} \cdots \frac{d\mathbf{p}'_1}{2p'_{10}} \cdots = 1. \tag{7}$$

The transition probability W can then be written as

$$\begin{aligned} W = \int & \zeta_m(\mathbf{p}'_1 \cdots \mathbf{p}'_m, \mathbf{p}_1 \cdots \mathbf{p}_m) F_n(\mathbf{q}_1 \cdots \mathbf{q}_n, \mathbf{q}'_1 \cdots \mathbf{q}'_n) \\ & \times T_{mn}(\mathbf{p}_1 \cdots \mathbf{p}_m, \mathbf{q}_1 \cdots \mathbf{q}_n) \\ & \times T^*_{mn}(\mathbf{p}'_1 \cdots \mathbf{p}'_m, \mathbf{q}'_1 \cdots \mathbf{q}'_n) \\ & \times \prod_{i=1}^{m} \frac{d\mathbf{p}_i}{2p_{10}} \prod_{i=1}^{n} \frac{d\mathbf{q}_i}{2q_{10}} \prod_{i=1}^{m} \frac{d\mathbf{p}'_i}{2p'_{10}} \prod_{i=1}^{n} \frac{d\mathbf{q}'_i}{2q'_{10}}. \end{aligned} \tag{8}$$

One should keep in mind that the meaning of the right-hand side of Eq. (8), where products of distributions have been written, is nothing else but the right-hand side of Eq. (4). However, we will in the following make further hypotheses on the kernels involved and use approximations which will explain the use of Eq. (8).

B. Energy–Momentum Conservation of the S Matrix

The property (P) which is considered here is Poincaré invariance. Let us assume that it holds in S-matrix theory for any given initial and final states and every element (a, Λ) of the Poincaré group

$$W(a, \Lambda) = W. \tag{9}$$

It implies the existence of a phase $\theta(a, \Lambda)$ such that

$$U(a, \Lambda) T U(a, \Lambda)^{-1} = e^{i\theta(a,\Lambda)} T. \tag{10}$$

$U(a, \Lambda)$ is the representation of the Poincaré group. Equation (10) is obtained using the theorem that two linear bounded operators such that $\langle f| A |q\rangle = 0 \Leftrightarrow \langle f| B |q\rangle = 0$, for all (f, q), are proportional. The modulus of the proportionality constant is unity here.

[1] E. H. Wichmann and J. H. Crichton, Phys. Rev. **132**, 2788 (1963).

[2] J. R. Taylor, Phys. Rev. **142**, 1236 (1966). Other interesting aspects of the cluster decomposition are discussed in M. Froissart and J. R. Taylor, "Cluster Decomposition and the Spin Statistics Theorem in S-matrix Theory," Princeton University preprint, 1966.

The phase θ, being a representation of dimension one of the Poincaré group, is a constant. Thus,

$$[U, T] = 0. \tag{11}$$

Let us note that a postulate concerning only translational invariance (of the transition probability) would not be sufficient to get a similar result (with U being a representation of the translations).

Equation (11) implies, in particular, the "energy–momentum conservation" of the S matrix. A precise definition of what is meant in general by energy–momentum conservation of an operator and its relation with translational invariance of this operator is to be found in Ref. 3.

The case of a Fock space and of the S matrix is a special one.

If we look at the properties induced for the matrix elements, Eq. (11) implies that the matrix elements T_{mn} can be written as a product of a global δ function of "energy–momentum conservation" by a kernel t_{mn} defined on the corresponding hyperplane:

$$T_{mn}(\mathbf{p}_1 \cdots, \mathbf{q}_1 \cdots) = t_{mn}\delta\left(\sum_{i=1}^{m} p_i - \sum_{i=1}^{n} q_i\right). \tag{12}$$

This result is obtained by considering the quantity:

$$T_{mn}^{(\varphi)}(a) = \int T_{mn}(\mathbf{p}_1 \cdots, \mathbf{q}_1 \cdots)\varphi(\mathbf{p}_1 \cdots, \mathbf{q}_1 \cdots) \times \exp\left[ia(\textstyle\sum p_i - \sum q_i)\right]\pi\, d\mathbf{p}_i\, \pi\, d\mathbf{q}_i.$$

Taking its derivative with respect to a yields

$$\frac{\partial T^{(\varphi)}}{\partial a_i} = 0, \quad i = 0, 1, 2, 3, \tag{13}$$

$$\left(\sum_{i=1}^{m} p_i - \sum_{i=1}^{n} q_i\right)T_{mn} = 0, \tag{14}$$

which yields Eq. (12). As a matter of fact, we get formula (12) only when the distribution kernel T_{mn} is restricted to the dense subspace of test functions with supports such that all velocities cannot be equal all together.

Conversely, assuming energy–momentum conservation of the S matrix, we get translational invariance of the S matrix, of the transition amplitudes, and thus of the transition probabilities for all initial and final states.

If the assumption is that the T-matrix elements satisfy Eq. (12), it yields translational invariance of the transition amplitudes (and probabilities), at least for a dense subspace of states (which depends on the nature of the t_{mn}).

C. Cluster Property of the S Matrix

One deals in a similar way with the concept of separate interactions.

As in the classical case, it is assumed that the main contribution to the transition probability, when subgroups of initial and final particles are taken away through 4-vectors $a, b, \cdots$, is obtained by calculating the product of partial transition probabilities.

What is meant by main "contribution" is made precise by Taylor[2] as a condition of uniform convergence in $|\mathbf{a}^2 + a_0^2|, |\mathbf{b}^2 + b_0^2|, \cdots$, for $|\mathbf{a}^2 + a_0^2| \to +\infty$, $|\mathbf{b}^2 + b_0^2| \to +\infty, \cdots$. He is then able to show that it implies a factorization property of the transition amplitudes.

As emphasized by Wichmann and Crichton,[1] then Williams,[3] we can, independently of the property stated above, consider a cluster parameterization of the S matrix (which is just a combinational mechanism):

$$T_{mn} = \sum_{I} \prod_{i} T^{c}_{m_i n_i}, \tag{15}$$

where I is any decomposition of the set m, n into subsets.

A result by Williams[3] tells us that the T^c_{mn} parameters are also bounded operators, as are the T_{mn}. In this special case, they also conserve "energy–momentum" as do the T_{mn} operators and their kernels can also be written as the product of a δ function of "conservation of energy–momentum" with a kernel defined on the corresponding hyperplane:

$$T^{c}_{mn}(\mathbf{p}_1 \cdots \mathbf{p}_m, \mathbf{q}_1 \cdots \mathbf{q}_n) = t^{c}_{mn}\delta\left(\sum_{1}^{m} p_i - \sum_{1}^{n} q_i\right). \tag{16}$$

The factorization property of T_{mn} is then equivalent to a further property of the connected amplitudes: if subgroups of initial and final particles are taken away, the amplitude of the matrix T^c_{mn} goes to zero.

It may seem too strong to consider the factorization property for all initial and final states and some authors[1,2] prefer to consider it only for subspaces of states—for instance the subspaces $\mathfrak{D}$ or $\mathcal{S}$ (of test functions of distributions or temperate distributions) of $L^2(R^3)$. The special conditions used to obtain the classical formulas are, in the usual cases, still more restrictive. The equivalent property of the matrix T^c_{mn} stated above refers to the subspace considered.

In all cases, the T^c_{mn} kernels have the form given in Eq. (16) and, in particular, the t^c_{mn} kernels do not contain any δ function of partial conservation of energy–momentum (nor any derivative of δ, of course). Further hypotheses on these kernels will be studied in the following.

D. One-Particle Singularities

Let us consider a scattering involving initial particles A, B, C and final particles A_1, B_1, C_1. The kinematical

[3] D. N. Williams, J. Math. Phys. **8**, 1807 (1967).

and other (superselection rules, etc.) conditions allow the possibility of partial scatterings $A + B \to A_1 + M$, $M + C \to B_1 + C_1$, for some particle M—all other partial scatterings of this type being forbidden.

If particles C, B_1, C_1 are taken away with a timelike 4-vector ρ ($\rho_0 > 0$) the main contribution to the classical transition probability is obtained through a formula corresponding to successive scatterings $A + B \to A_1 + M$, $M + C \to B_1 + C_1$.

One first determines the state of the real intermediate particle M, which may be either stable or not. The probability of the second scattering is then calculated and gives the final result.

In that case, the description of the intermediate particle state is involved. Let us note that, in the usual classical situations, the two scatterings can be well enough localized in space–time and the intermediate particle M can be considered as freely propagating when the second scattering takes place.

If it is, furthermore, a stable particle, the above property of the transition probability can be stated independently of the description of the states.

The following property (P) would then be assumed in S-matrix theory: the main contribution for large ρ_0 to the transition probability of the scattering $A + B + C \to A_1 + B_1 + C_1$ is obtained by considering a first scattering $A + B \to A_1 + M$, evaluating the final state of particle M, reinterpreting it as an initial state, and calculating the transition probability of a second scattering $M + C \to B_1 + C_1$.

One uses then the same line of thought as in Secs. II.B and II.C. What is meant by main contribution can be made precise with the help of more or less strong hypotheses which imply the existence of the well-known propagator in connected S-matrix elements.[4–8]

Conversely, one may assume a polelike behavior of the S-matrix elements plus some related hypotheses and find back the above property of the transition probability.[7–9]

One may also assume a Landau-type behavior of the S-matrix elements. Simple qualitative arguments[10] are hints which indicate that Landau singularities in the physical region may correspond to some related physical processes. Then, it is also possible to deduce some related property of the transition amplitude,[7] thus the transition probability.

We give an account of such attempts in Appendix A.

However, the hypotheses used, either in the precise statement of property (P), or together with the polelike or Landau-type behavior to get some property of the transition amplitude, are rather arbitrary and not unique. On the other hand, even if we assume any of them, the classical formulas have still to be obtained.

We will then, assuming the polelike behavior in a weak form, directly show how it leads, under special conditions, to the classical description and formulas.[9]

III. CORRESPONDENCE BETWEEN QUANTUM-MECHANICAL AND CLASSICAL DESCRIPTIONS OF STATES

Section III.A is devoted to the analysis of the classical description of particle states and their measurement apparatus through probability densities and measurement efficiencies in phase space.

Following Wigner,[11,12] we introduce the density and efficiency functions associated in quantum mechanics to the density and efficiency matrices. Invariant density and efficiency functions are also introduced. The general properties of such functions are studied in Sec. III.B. Cases where the Wigner functions are actually positive and smaller than one are given. In all cases, it is shown that these functions, once they have been smoothed out over a phase space region of dimensions larger or equal to one are always positive and smaller than one (i.e., enjoy a property required for the classical probability density or measurement efficiency).

Invariant density or efficiency functions are shown to enjoy a similar property in the approximation where the quantity $1/m$ is negligible compared to the space diameter of the phase-space region considered. Note that $1/m = \hbar/mc$. In the nonrelativistic case, the condition is then always satisfied ($c = +\infty$).

These properties are already a first hint that such functions are actually good candidates for a correspondence between quantum-mechanical and classical descriptions.

In all what follows, a situation will be said to be of a classical type if the density or efficiency functions involved can be replaced with a good approximation by functions enjoying the properties of classical probability density or measurement efficiency. We also say that the classical approximation can be used, and we obtain a classical-type formula.

[4] G. Wanders, Helv. Phys. Acta **38**, 142 (1965).
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[10] S. Coleman and R. E. Norton, Nuovo Cimento **38** (1965).
[11] E. P. Wigner, Phys. Rev. **40**, 749 (1932).
[12] For a review of the applications of the phase-space formulation of quantum-statistical mechanics, see H. Mori, J. Oppenheim, and J. Ross, in *Studies in Statistical Mechanics*, J. de Boer and G. E. Uhlenbeck, Eds. (North-Holland Publ. Co., Amsterdam, 1962), Vol. 1, p. 272–298. It is a kind of work analogous to what is done in our work in the nonrelativistic case when equations of evolution with time are used.

In Sec. III.C, it is shown that density or efficiency functions are themselves of a classical type, without smoothing, if they are slowly varying over a phase-space region of dimensions large compared to unity. A similar property holds for the invariant functions if, furthermore, $1/m$ is small compared to the space diameter of a region for which the above property holds.

All these results are new hints that the correspondence is a good one. We will use it in the following parts and the fact that it will allow one to obtain classical-type formulas in many cases of interaction processes proves that the whole scheme is consistent.

A. Classical Description

In classical formalism, the state of a particle is described by giving its current $j_\mu(P, x)$, where j_0 is the probability density of finding the particle at point x with momentum P and $\mathbf{j}$ is the current density.

For a freely propagating stable particle of mass m, the following properties hold:

$$\partial^\mu j_\mu = 0. \tag{17a}$$

The current j_μ is proportional to P_μ and we define the current intensity $j(P, x)$ through

$$j(P, x) = j_\mu / 2P_\mu . \tag{17b}$$

The quantity $j(P, x)$ has the form

$$j(P, x) = g(\mathbf{P}, \mathbf{x} - (\mathbf{P}/P_0)x_0)\delta(P^2 - m^2)\theta(P_0). \tag{17c}$$

The function g is the probability density in phase space and contains all the information [the fact that the mass is known to be m and the particle is known to be freely propagating have been used in writing (17c)].

A final property is

$$\int j_0(P, x)\, dP\, d\mathbf{x} = \int g(\mathbf{P}, \mathbf{y})\, d\mathbf{P}\, d\mathbf{y} = 1. \tag{17d}$$

The function g defined above is a positive measure (as well as j).

A "pure case" is

$$g(\mathbf{P}, \mathbf{y}) = \delta(\mathbf{P} - \mathbf{P}_0)\delta(\mathbf{y} - \mathbf{y}_0).$$

The description of a measurement apparatus of a particle is done in the same way by defining its efficiency $E(P, x)$ for detecting a particle at point x with momentum P.

With similar hypotheses, E has the form

$$E(P, x) = \epsilon(\mathbf{P}, \mathbf{x} - (\mathbf{P}/P_0)x_0)\delta(P^2 - m^2)\theta(P_0), \tag{18a}$$

where the quantity ϵ is the measurement efficiency in phase space.

For every given quantity g satisfying Eqs. (17), ϵ has to satisfy

$$0 \leq \int \epsilon(\mathbf{P}, \mathbf{y}) g(\mathbf{P}, \mathbf{y})\, d\mathbf{P}\, d\mathbf{y} \leq \int g(\mathbf{P}, \mathbf{y})\, d\mathbf{P}\, d\mathbf{y} = 1. \tag{18b}$$

It seems "physically reasonable" to consider that ϵ belongs to the class of Borelian functions satisfying

$$0 \leq \epsilon(\mathbf{P}, \mathbf{y}) \leq 1. \tag{18c}$$

One could choose a more general definition, mathematically speaking [we only want $\int \epsilon g$ to be defined for all measures g].

Physically speaking, some authors prefer to restrict ϵ to be a continuous function. An apparatus with efficiency one inside a box and zero outside this box is then excluded.

Information theory[13] allows one to determine the quantity g (or ϵ) corresponding to a given information. The quantity

$$\int g(\mathbf{P}, \mathbf{x}) \ln g(\mathbf{P}, \mathbf{x})\, d\mathbf{P}\, d\mathbf{x}$$

has to be made minimal with respect to the given information.

If we know a set of quantities

$$r_i = \int g(\mathbf{P}, \mathbf{x}) R_i(\mathbf{P}, \mathbf{x})\, d\mathbf{P}\, d\mathbf{x}$$

for a set of functions R_i, the solution has the form

$$g(\mathbf{P}, \mathbf{x}) \propto \exp\left[-\sum \lambda_i R_i(\mathbf{P}, \mathbf{x})\right]. \tag{19}$$

For instance, if we know the position and momentum of the particle to be $\mathbf{P}_0$ and $\mathbf{x}_0$ with root-mean-square deviations A_x, A_p, there is a solution for all $\mathbf{P}_0$, $\mathbf{x}_0$, A_x, A_p:

$$g_0(\mathbf{P}, \mathbf{x}) = \frac{1}{(2\pi)^3 (A_x A_p)^3} \exp\left[-\frac{1}{2}\left(\frac{\mathbf{x} - \mathbf{x}_0}{A_x}\right)^2\right] \times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{P} - \mathbf{P}_0}{A_p}\right)^2\right]. \tag{20}$$

More generally, if we know the distribution in momentum and position to be a positive measure $\mu(\mathbf{P}, \mathbf{x})$, with rms errors A_x, A_p on the measurement of position and momentum, the solution is the convolution:

$$g(\mathbf{P}, \mathbf{x}) = \mu(\mathbf{P}, \mathbf{x}) * \tau_{A_x}(\mathbf{x})\tau_{A_p}(\mathbf{P}), \tag{21a}$$

where

$$\tau_{A_x}(\mathbf{x}) = \frac{1}{(2\pi^3)^{\frac{1}{2}}} \frac{1}{A_x^3} \exp\left(-\frac{1}{2}\frac{\mathbf{x}^2}{A_x^2}\right). \tag{21b}$$

[13] See, for instance, A. Katz, *Principles of Statistical Mechanics, The Information Theory Approach* (the Weizmann Institute Lectures, 1963).

B. Wigner-like Density and Efficiency Functions

We go back to the quantum-mechanical description of one-particle states and measurement apparatus by means of density or efficiency matrices and we associate to them the following quantities:

$$g_W(\mathbf{P}, \mathbf{x}) = \int \frac{\zeta(\mathbf{p}, \mathbf{p}')}{(2p_0)^{\frac{1}{2}}(2p_0')^{\frac{1}{2}}} \exp\,[i(\mathbf{p} - \mathbf{p}')\mathbf{x}] \times \delta(\tfrac{1}{2}(\mathbf{p} + \mathbf{p}') - \mathbf{P})\, d\mathbf{p}\, d\mathbf{p}', \tag{22}$$

$$j_I(P, x) = \int \zeta(\mathbf{p}, \mathbf{p}') \exp\,[i(p - p')x] \times \delta(\tfrac{1}{2}(p + p') - P) \frac{d\mathbf{p}}{2p_0} \frac{d\mathbf{p}'}{2p_0'}, = j_I(P, \mathbf{x} - (\mathbf{P}/P_0)x_0) \tag{23}$$

$$j_F(P, x) = \left[\int j_I(\lambda P, x)\, d\lambda\right] \delta(P^2 - m^2)\theta(P_0) = g_F(\mathbf{P}, \mathbf{x} - (\mathbf{P}/P_0)x_0)\delta(P^2 - m^2)\theta(P_0), \tag{24}$$

and similar quantities ϵ_W, E_I, E_F associated with the efficiency matrix F.

As a matter of fact, the quantities to be compared with the classical probability density are $(2\pi)^{-3}$ times g_W or j_I, j_F, g_F. The quantities to be compared with the classical measurement efficiency are ϵ_W, E_I, E_F, ϵ_F.

All the kernels involved are temperate distributions, which give a precise meaning to the Fourier transformations considered as temperate distributions.

The function g_W is the usual Wigner function.[11] The functions j_I and j_F are more suited in the relativistic case for reasons of covariance. The function j_F formally has the same form as in the classical case [Eq. (17c)].

Our purpose is now to study the properties of these various quantities in Sec. III.B and to show how they behave under special conditions in Sec. III.C. We first begin by studying the properties of g_W and ϵ_W for the sake of clarity.

1. General Properties of Wigner Functions

The quantities g_W, introduced by Wigner,[12] and ϵ_W are, as stated above, well-defined distributions. As for g_W, it is also a square-integrable function due to Eq. (7). As is well known, these real quantities are not always positive.

To find which ζ and which g_W correspond to a given information on a system, one makes the quantity $\mathrm{Tr}\,\zeta \ln \zeta$ minimal according to the given information.[13]

Cases where the Wigner function is positive. We first study cases where g_W is actually positive.

Take the special case where the information comes from "measurements of position and momentum" of the particle. For instance, as in the classical case studied above, we know the position $\mathbf{x}_0$, the momentum $\mathbf{P}_0$ with rms errors A_x and A_p or, more precisely,

$$\begin{aligned} \mathrm{Tr}\,\zeta \mathbf{X}_{0p} &= \mathbf{x}_0, \\ \mathrm{Tr}\,\zeta \mathbf{P}_{0p} &= \mathbf{P}_0, \\ \mathrm{Tr}\,\zeta(\mathbf{X}_{0p} - \mathbf{x}_0)^2 &= A_x^2, \\ \mathrm{Tr}\,\zeta(\mathbf{P}_{0p} - \mathbf{P}_0)^2 &= A_p^2, \end{aligned} \tag{25}$$

where $\mathbf{X}_{0p}$ is the usual Newton–Wigner operator.

The Wigner function is then found to be formally identical to the probability density of the similar classical case

$$g_W(\mathbf{P}, \mathbf{x}) = \frac{1}{(2\pi)^3} \frac{1}{A_x^3} \exp\left[-\frac{1}{2}\left(\frac{\mathbf{x} - \mathbf{x}_0}{A_x}\right)^2\right] \frac{1}{A_p^3} \times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{P} - \mathbf{P}_0}{A_p}\right)^2\right]. \tag{26}$$

It is the Wigner function of a density matrix ζ if and only if $A_x A_p \geq \frac{1}{2}$:

$$\zeta = \frac{1}{(2\pi)^3} \frac{1}{(A_x' A_p')^3} \times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{P}_{0p} - \mathbf{P}_0}{A_p'}\right)^2 - \frac{1}{2}\left(\frac{\mathbf{X}_{0p} - \mathbf{x}_0}{A_x'}\right)^2\right], \tag{27}$$

where

$$\left(\frac{A_x}{A_x'}\right)^2 = \left(\frac{A_p}{A_p'}\right)^2 = \frac{1}{A_x' A_p' \tanh\,(1/A_x' A_p')}.$$

Thus, the Wigner function is actually positive. More generally, if we know a "phase-space distribution" μ, with rms errors A_x, A_p in the measurements of position and momentum ($A_x A_p \geq \frac{1}{2}$), the Wigner function takes the form

$$g_W(\mathbf{P}, \mathbf{x}) = \mu(\mathbf{P}, \mathbf{x}) * \tau_{A_x}(\mathbf{x})\tau_{A_p}(\mathbf{P}), \tag{28}$$

where

$$\tau_{A_x}(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \frac{1}{A_x^3} \exp\left(-\frac{1}{2}\frac{\mathbf{x}^2}{A_x^2}\right).$$

A similar result would be obtained for ϵ_W.

The following result then holds: if μ satisfies the properties required from a classical probability density (positive measure of sum one) (respectively, the properties of a measurement efficiency $0 \leq \mu \leq 1$), then g_W (respectively, ϵ_W) is actually the Wigner function of a density matrix (respectively an efficiency matrix).

General properties. As is well known, even if the Wigner function is not positive, the marginal probabilities of g_W in $\mathbf{x}$ or $\mathbf{P}$ are positive (and equal to the quantum-mechanical probability in $\mathbf{x}$ or $\mathbf{P}$).

The most interesting property is the following: the function g_W (respectively, ϵ_W) once smoothed out over any phase-space region of dimensions larger than or equal to unity, is always positive and smaller than one—i.e., satisfies the property required from a classical measurement efficiency

$$0 \leq \epsilon_W(\mathbf{P}, \mathbf{x}) * \tau_{B_x}(\mathbf{x})\tau_{B_p}(\mathbf{P}) \leq 1, \quad \text{for} \quad B_x B_p \geq \tfrac{1}{2}. \tag{29}$$

The discussion is given in Appendix B.

Another well-known property concerning measurement results is the following:

$$\operatorname{Tr} \zeta F = \int g_W(\mathbf{P}, \mathbf{x})\epsilon_W(\mathbf{P}, \mathbf{x})\, d\mathbf{P}\, d\mathbf{x}. \tag{30}$$

This is, then, a formally classical-type formula.

We recall however that, as is well known, the Wigner function—which is generally defined with the same Wigner transformation as used in the special cases of the density or efficiency matrix—associated with a product of two bounded operators, is different from the product of the Wigner functions:

$$(AB)_W(\mathbf{P}, \mathbf{x}) = \int (A)_W(\mathbf{P}', \mathbf{x}')(B)_W(\mathbf{P}'', \mathbf{x}'') \times \exp\left[2i \begin{vmatrix} 1 & \mathbf{P} & \mathbf{x} \\ 1 & \mathbf{P}' & \mathbf{x}' \\ 1 & \mathbf{P}'' & \mathbf{x}'' \end{vmatrix}\right] d\mathbf{P}'\, d\mathbf{P}''\, d\mathbf{x}'\, d\mathbf{x}''. \tag{31}$$

It is also different from $(BA)_W$ in general.

Other special cases. In the following we consider particular cases where g_W is slowly varying in intervals of the order of some quantity A_x in $\mathbf{x}$ or A_p in $\mathbf{P}$, or both. The specific form will be

$$g_W(\mathbf{P}, \mathbf{x}) = h_W(\mathbf{P}, \mathbf{x}) * \tau_{A_x}(\mathbf{x}) \tag{32}$$

(or similarly in $\mathbf{P}$) where h is some distribution.

We will then call A_x the position deviation (respectively, A_p the momentum deviation). In fact, the probability of finding the particle at point $\mathbf{x}_0$ with an apparatus measuring with infinite precision at that point is

$$W(\mathbf{x}_0) = \int g_W(\mathbf{P}, \mathbf{x})\delta(\mathbf{x} - \mathbf{x}_0)\, d\mathbf{P}\, d\mathbf{x} = \int g_W(\mathbf{P}, \mathbf{x}_0)\, d\mathbf{P}$$

and is thus slowly varying with $\mathbf{x}_0$ in an interval of the order of A_x. A similar argument holds for a quantity ϵ_W of form (30). We say here that the probability of detecting a particle at point $\mathbf{x}_0$ with rms error B_x and, say, momentum $\mathbf{P}_0$ with rms error B_p is

$$W = [h(\mathbf{P}, \mathbf{x}) * \tau_{B_p}(\mathbf{P})\tau_{A_x'}(\mathbf{x})](\mathbf{P}_0, \mathbf{x}_0),$$

where

$$A_x' = (A_x^2 + B_x^2)^{\frac{1}{2}}.$$

Then, however small we choose B_x, A_x' is larger than A_x.

2. *General Properties of Invariant Density or Efficiency Functions*

As already stated, the functions j_I and j_F are covariant. Furthermore, j_F enjoys the property expressed by Eq. (17c). We will be interested in this section in the function g_F.

It is a covariant function, as opposed to g_W, but it does not enjoy anymore the properties given in Eqs. (29) and (30). We will now show that it almost enjoys in some sense the property expressed in Eq. (29) for g_W. The invariant density or efficiency functions smoothed out over a phase-space region of dimensions larger than or equal to one, are positive and smaller than one, in the approximation that the space diameter of the region considered, is taken large compared to the quantity $1/m$.

Explicit calculations give

$$j_I(P, \mathbf{y}) = \int \zeta(\mathbf{p}, \mathbf{p}') \exp[i(\mathbf{p} - \mathbf{p}')\mathbf{y}] \times \delta\left(\frac{\mathbf{p} + \mathbf{p}'}{2} - \mathbf{P}\right)\frac{2(p_0 + p_0')}{2p_0p_0'}\,\theta(P_0) \times \delta\left(P^2 - m^2 + \frac{\mathbf{u}^2}{4} - \frac{(\mathbf{vu})^2}{4}\right) d\mathbf{p}\, d\mathbf{p}', \tag{33a}$$

where

$$\mathbf{v} = \mathbf{P}/P_0, \qquad \mathbf{u} = \mathbf{p} - \mathbf{p}'.$$

As for g_F, it can be written as

$$g_F(\mathbf{P},\mathbf{y}) = \int \xi(\mathbf{P},\mathbf{u}) \exp(i\mathbf{uy})\, d\mathbf{u}, \tag{33b}$$

with

$$\xi(\mathbf{P}, \mathbf{u}) = (1/\lambda_0)\bar{\zeta}(\lambda_0\mathbf{P}, \mathbf{u}),$$

$$\lambda_0 = \left(1 + \frac{\mathbf{u}^2 - (\mathbf{vu})^2}{4m^2}\right)^{\frac{1}{2}},$$

$$\bar{\zeta}\left(\frac{\mathbf{p} + \mathbf{p}'}{2}, \mathbf{p} - \mathbf{p}'\right) = \zeta(\mathbf{p}, \mathbf{p}')\frac{p_0 + p_0'}{2p_0p_0'}.$$

To prove the result, we first obtain a slight extension of Eq. (29) for the case when B_x depends on the momentum.

Limiting the proof to the case $B_xB_p = \frac{1}{2}$, one writes the inequality,

$$0 \leq \langle\chi_0|\, F\,|\chi_0\rangle \leq \langle\chi_0\,|\,\chi_0\rangle,$$

for the minimal wave packet:

$$\chi_0(\mathbf{p}) = \frac{(2p_0)^{\frac{1}{2}}}{(2\pi)^{\frac{3}{2}}} \exp(i\mathbf{p}\mathbf{x}_0) \times \exp\left(-\frac{1}{2}\frac{(\mathbf{p} - \mathbf{P}_0)^2}{4} B_x^2(\mathbf{P}_0)\right) B_x^{\frac{3}{2}}(\mathbf{P}_0),$$

which gives the general result

$$0 \leq \int \epsilon_W(\mathbf{P}, \mathbf{x}) \frac{1}{(2\pi)^3} \exp\left[-\frac{1}{2}\left(\frac{\mathbf{P}-\mathbf{P}_0}{B_p(\mathbf{P}_0)}\right)^2\right] \times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{x}-\mathbf{x}_0}{B_x(\mathbf{P}_0)}\right)^2\right] d\mathbf{P}\, d\mathbf{x} \leq 1.$$

It is now sufficient to prove that at the approximation stated, ϵ_W can be replaced by ϵ_F. We will use the special choice

$$B_x(\mathbf{P}_0) = B_{x0}(1 - \mathbf{v}_0^2)^{-\frac{1}{2}}.$$

We consider the quantity

$$N(\zeta) = \int [\xi(\mathbf{P}, \mathbf{u}) - \hat{\zeta}(\mathbf{P}, \mathbf{u})] \exp(i\mathbf{u}\mathbf{y}_0) B_x^3(\mathbf{P}_0) \times \exp[-\tfrac{1}{2}(\mathbf{P}-\mathbf{P}_0)^2 B_x^2(\mathbf{P}_0)] \times \exp[-B_x^2(\mathbf{P}_0)\mathbf{u}^2]\, d\mathbf{P}\, d\mathbf{u},$$

where

$$\hat{\zeta}(\mathbf{P}, \mathbf{u}) = \zeta(\mathbf{p}, \mathbf{p}')[(2p_0)^{\frac{1}{2}}(2p_0')^{\frac{1}{2}}]^{-1},$$

$$\xi(\mathbf{P}, \mathbf{u}) = \frac{1}{\lambda_0} \hat{\zeta}(\lambda_0 \mathbf{P}, \mathbf{u}) \frac{p_0 + p_0'}{2(p_0 p_0')^{\frac{1}{2}}}.$$

A tedious but straightforward evaluation leads to the result that $|N(\zeta)|$ is of the order of $|P(1/m^2 B_x^2 B_p)|$ (which is smaller than $1/mB_{x0}$).

It is obtained, by using

$$\lambda_0 = 1 + \mathcal{O}([mB_x(\mathbf{P}_0)]^{-2})$$

$$\frac{p_0 + p_0'}{2(p_0 p_0')^{\frac{1}{2}}} = 1 + \mathcal{O}([mB_x(\mathbf{P}_0)]^{-3})$$

$$\frac{P}{[mB_x(\mathbf{P}_0)]^2} = \frac{P_0}{[mB_x(\mathbf{P}_0)]^2} + \mathcal{O}\left(\frac{1}{B_x(\mathbf{P}_0)} \frac{1}{[mB_x(\mathbf{P}_0)]^2}\right).$$

Because of the exponential factor in the integrand, all correcting quantities are well defined.

C. Classical Limit of Wigner-like Functions

1. Classical Limit of the Usual Wigner Functions

A density or an efficiency function is expected to be of a classical type if the probabilistic aspect due to insufficient data (with respect to phase space) is such that essentially all information on the quantum level is lost.

If the correspondence between classical and S-matrix descriptions of states which has been established by means of density and efficiency functions is good, these functions should then enjoy without smoothing the properties required from the corresponding classical functions with a good approximation. We emphasize that only a subclass of the classical functions will be obtained, as is physically the case.

A qualitative requirement which is expected is a slow variation of the density or efficiency functions over phase-space regions of dimensions large compared to unity.

More generally, a qualitative requirement for a situation to be of a classical type is that some product $|(\nabla_x f)(\nabla_p g)|$ of some functions involving f and g, should be large compared to unity.

In this section, we show, in some simple cases, that this qualitative requirement can be made precise in a satisfactory way. We study the case of a Wigner function itself, the case of a product of two Wigner functions, and, finally, different classical-type situations corresponding to measurements.

Classical limit of a Wigner function. Let us first consider the special simple case of the density matrix ζ_0 defined in Eq. (27).

$$\zeta_0 = \frac{1}{(2\pi)^3} \frac{1}{(A_x' A_p')^3} \times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{P}_{0p} - \mathbf{P}_0}{A_p'}\right)^2 - \frac{1}{2}\left(\frac{\mathbf{X}_{0p} - \mathbf{x}_0}{A_x'}\right)^2\right],$$

$$g_0(\mathbf{P}, \mathbf{x}) = \frac{1}{(2\pi)^3} \frac{1}{(A_x A_p)^3} \times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{P}-\mathbf{P}_0}{A_p}\right)^2 - \frac{1}{2}\left(\frac{\mathbf{X}-\mathbf{x}_0}{A_x}\right)^2\right],$$

$$\left(\frac{A_x'}{A_x}\right)^2 = \left(\frac{A_p'}{A_p}\right)^2 = 2A_x' A_p' \tanh \frac{1}{2A_x' A_p'}.$$

The Wigner function g_0 is always positive (and less than one), but for instance the Wigner function $(\zeta_0^2)_W(\mathbf{P}, \mathbf{x})$ associated with ζ_0^2 is completely different in general from $g_0^2(\mathbf{P}, \mathbf{x})$.

However, if we consider a sequence of such density matrices such that $A_x A_p$ goes to infinity, the following results hold:

$$\frac{A_x}{A_x'} = 1 + \mathcal{O}\left(\frac{1}{A_x A_p}\right), \quad (34a)$$

$$\frac{A_p}{A_p'} = 1 + \mathcal{O}\left(\frac{1}{A_x A_p}\right), \quad (34b)$$

$$|(\zeta_0^2)_W(\mathbf{P}, \mathbf{x}) - g_0^2(\mathbf{P}, \mathbf{x})| = \mathcal{O}\left(\frac{1}{A_x A_p}\right). \quad (34c)$$

Equation (34c) is easily obtained due to the simple form of ζ_0.

We now study the general case when the Wigner function is slowly varying over some phase-space region, with a "space deviation" A_x and "momentum deviation" A_p. The specific form is thus

$$\epsilon_W(\mathbf{P}, \mathbf{x}) = \mu(\mathbf{P}, \mathbf{x}) * \tau_{A_p}(\mathbf{P}) \tau_{A_x}(\mathbf{x}), \quad (35)$$

where μ is some function such that ϵ_W is actually the Wigner function of a density or efficiency matrix. It is sufficient to limit ourselves to that case as we

consider the limit $A_xA_p \to \infty$ in the following. If it were a more general distribution, a small part of the convolutions would be taken out to smooth it.

It includes the cases already studied where μ was positive, but also all other possible cases.

Owing to Eq. (29), one has, for any B_x, B_p ($B_xB_p \geq \frac{1}{2}$),

$$0 \leq \epsilon_W * \tau_{B_p}(\mathbf{P})\tau_{B_x}(\mathbf{x}) = \mu * \tau_{C_p}(\mathbf{P})\tau_{C_x}(\mathbf{x}) \leq 1, \tag{36a}$$

$$C_p = A_p\left[1 + \left(\frac{B_p}{A_p}\right)^2\right]^{\frac{1}{2}},$$

$$C_x = A_x\left[1 + \left(\frac{B_x}{A_x}\right)^2\right]^{\frac{1}{2}}.$$

If we consider a sequence of Wigner functions

$$(\epsilon_W)_{A_x,A_p}(\mathbf{P}, \mathbf{x}) = \mu_{A_x,A_p}(\mathbf{P}, \mathbf{x}) * \tau_{A_p}(\mathbf{P})\tau_{A_x}(\mathbf{x}),$$

such that A_pA_x goes to infinity, and μ_{A_p,A_x} is a set of uniformly bounded functions, it is easily shown that

$$|(\epsilon_W)_{A_p,A_x}(\mathbf{P}, \mathbf{x}) - (\epsilon_W)_{A_p,A_x} * \tau_{B_p}(\mathbf{P})\tau_{B_x}(\mathbf{x})| = \mathcal{O}((A_xA_p)^{-1}), \tag{36b}$$

with

$$B_x = A_x(A_xA_p)^{-\frac{1}{2}},$$
$$B_p = A_p(A_xA_p)^{-\frac{1}{2}},$$

Equation (36b), together with Eq. (36a), proves that, actually for large A_xA_p, the Wigner function ϵ_W becomes positive and less than unity. (It is always a C^∞ function, because of the convolutions.)

Two special limit cases can be mentioned, namely, cases when the Wigner function only depends on the position or the momentum variables, corresponding to measurement apparatus only detecting position or momentum.

The special form of the efficiency matrix F is such that

$$F_W(\mathbf{p}, \mathbf{p}') = A(\tfrac{1}{2}(\mathbf{p} + \mathbf{p}')),$$
$$\epsilon_W(\mathbf{P}, \mathbf{x}) = A(\mathbf{P}), \tag{37}$$

or

$$F_W(\mathbf{p}, \mathbf{p}') = B(\mathbf{p} - \mathbf{p}'),$$
$$\epsilon_W(\mathbf{P}, \mathbf{x}) = \tilde{B}(\mathbf{x}), \tag{38}$$

where $\tilde{B}$ is the Fourier transform of B.

In both cases, the condition $0 \leq F \leq 1$ is equivalent to $0 \leq \epsilon_W \leq 1$.

The property corresponding to Eq. (34b) in the general case will be a special case of the general result which will be obtained now.

Classical character with respect to each other of two Wigner functions. We consider here the Wigner function $(F_1F_2)_W(\mathbf{P}, \mathbf{x})$ associated with the product F_1F_2 of two density or efficiency matrices F_1, F_2, the Wigner function of each $\epsilon_{W,1}$, $\epsilon_{W,2}$ having the form given in Eq. (35), in general with different quantities $A_{p,1}$, $A_{x,1}$, and $A_{p,2}$, $A_{x,2}$:

$$\epsilon_{W,1}(\mathbf{P}, \mathbf{x}) = \mu_1 * \tau_{A_{p,1}}(\mathbf{P})\tau_{A_{x,1}}(\mathbf{x}),$$
$$\epsilon_{W,2}(\mathbf{P}, \mathbf{x}) = \mu_2 * \tau_{A_{p,2}}(\mathbf{P})\tau_{A_{x,2}}(\mathbf{x}).$$

We will then show that, for large products $A_{p,1}A_{x,2}$ and $A_{p,2}A_{x,1}$, the product of the Wigner functions $\epsilon_{W,1}(\mathbf{P}, \mathbf{x})$ $\epsilon_{W,2}(\mathbf{P}, \mathbf{x})$ becomes equal with a good approximation to the Wigner function $(F_1F_2)_W(\mathbf{P}, \mathbf{x})$. The result holds even if the Wigner functions $\epsilon_{W,1}$ and $\epsilon_{W,2}$ are not themselves of a classical type. We will say, generally speaking, that the two Wigner functions are formally of a classical type with respect to each other.

We assumed that μ_1 and μ_2 are uniformly bounded functions.

In fact, one has

$$(F_1F_2)_W(\mathbf{P}, \mathbf{x}) = \int \mu_1(\mathbf{P}_1, \mathbf{x}_1)\mu_2(\mathbf{P}_2, \mathbf{x}_2)\, d\mathbf{P}_1\, d\mathbf{x}_1\, d\mathbf{P}_2\, d\mathbf{x}_2 \frac{1}{(2\pi)^3(A_xA_p)^3}$$
$$\times \left\{\exp\left[-\frac{1}{2}\left(\frac{\mathbf{X}_{0p} - \mathbf{x}_1}{A'_{x,1}}\right)^2 - \frac{1}{2}\left(\frac{\mathbf{P}_{0p} - \mathbf{P}_1}{A'_{p,1}}\right)^2\right]\right.$$
$$\left.\times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{X}_{0p} - \mathbf{x}_2}{A'_{x,2}}\right)^2 - \frac{1}{2}\left(\frac{\mathbf{P}_{0p} - \mathbf{P}_2}{A'_{p,2}}\right)^2\right]\right\}_W(\mathbf{P}, \mathbf{x}). \tag{39}$$

A straightforward calculation gives

$$\left\{\exp\left[-\frac{1}{2}\left(\frac{\mathbf{X}_{0p} - \mathbf{x}_1}{A'_{x,1}}\right)^2 - \frac{1}{2}\left(\frac{\mathbf{P}_{0p} - \mathbf{P}_1}{A'_{p,1}}\right)^2\right]\right.$$
$$\left.\times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{X}_{0p} - \mathbf{x}_2}{A'_{x,2}}\right)^2 - \frac{1}{2}\left(\frac{\mathbf{P}_{0p} - \mathbf{P}_2}{A'_{p,2}}\right)^2\right]\right\}_W(\mathbf{P}, \mathbf{x})$$
$$= \frac{1}{(1 + K_{12}^2)^{\frac{1}{2}}(1 + K_{21}^2)^{\frac{1}{2}}}$$
$$\times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{P} - \mathbf{P}_1}{A_{p,1}}\right)^2 \frac{1}{1 + K_{12}^2}\right]$$
$$\times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{x} - \mathbf{x}_1}{A_{x,1}}\right)^2 \frac{1}{1 + K_{12}^2}\right]$$
$$\times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{x} - \mathbf{x}_2}{A_{x,2}}\right)^2 \frac{1}{1 + K_{21}^2}\right]$$
$$\times \exp\left[-\frac{1}{2}\left(\frac{\mathbf{P} - \mathbf{P}_2}{A_{p,2}}\right)^2 \frac{1}{1 + K_{21}^2}\right]$$
$$\times \exp\left[i\left(\frac{\mathbf{P}_2 - \mathbf{P}}{A_{p,2}} \frac{\mathbf{x} - \mathbf{x}_1}{A_{x,1}} \frac{K_{21}}{1 + K_{21}^2}\right.\right.$$
$$\left.\left. + \frac{K_{12}}{1 + K_{12}^2} \frac{\mathbf{P} - \mathbf{P}_1}{A_{p,1}} \frac{\mathbf{x} - \mathbf{x}_2}{A_{x,2}}\right)\right],$$

where

$$K_{12} = 1/A_{p,1}A_{x,2},$$
$$K_{21} = 1/A_{p,2}A_{x,1}.$$

Due to the above hypotheses, the result announced above holds in the following form:

$$|(F_1F_2)_W(\mathbf{P}, \mathbf{x}) - \epsilon_{W,1}(\mathbf{P}, \mathbf{x})\epsilon_{W,2}(\mathbf{P}, \mathbf{x})| = \mathcal{O}(K_{12}, K_{21}). \quad (40)$$

We have thus been able until now to study the case of classical-type Wigner functions and of two Wigner functions formally of a classical type with respect to each other. We deal now with measurement processes, as a first simple example.

We have given a precise characterization in the form of Eq. (35). A question is to what extent is it possible to generalize it. In the same line of thought as above, generalizations can be made by allowing A_p, A_x to depend on phase-space points. The momentum dependence can be easily given. A complete phase-space dependence is not quite easy, and not very useful (some more conditions on the variations of A_p, A_x as functions of $\mathbf{P}$ and $\mathbf{x}$ have to be given).

More generally, it is possible to write formally different "expansions of the Wigner functions in powers of h." What is sometimes stated as "taking the limit $\hbar = 0$" means in our formulation that terms of the kind $[(\nabla_x f)(\nabla_p g)]^{-1}$ would be assumed to be small enough to be negligible.

However, if it is formally possible, we do not know how to specify, in general, how the limit is obtained.

The characterization given in our text seems "physically reasonable."

Classical type formulas for measurements results. The general formula for a measurement result has been written in Eq. (30). We note that it is already a formally classical-type formula.

Cases for which we get classical-type formulas are all those for which the Wigner functions involved are actually positive (and less than one) or are of a classical type.

A simple example of another possible classical-type situation is exhibited as follows: assume that $g_W(\mathbf{P}, \mathbf{x})$ is negligible outside a sphere of diameter D and center $\mathbf{P}_a$ and that $\epsilon_W(\mathbf{P}, \mathbf{x})$ is slowly varying in an interval of the order of D in the variable $\mathbf{P}$. Different kinds of hypotheses can make the following rigorous.

An approximation for the quantity Tr ζF will be

$$\begin{aligned}\text{Tr } \zeta F &= \int g_W(\mathbf{P}, \mathbf{x})\epsilon_W(\mathbf{P}, \mathbf{x})\, d\mathbf{P}\, d\mathbf{x} \\ &\approx \int g_W^{\text{marg}}(\mathbf{x})\epsilon_W(\mathbf{P}_a, \mathbf{x})\, d\mathbf{x} \\ &= \int g_W^{\text{marg}}(\mathbf{x})\delta(\mathbf{P} - \mathbf{P}_a)\epsilon_W(\mathbf{P}, \mathbf{x})\, d\mathbf{P}\, d\mathbf{x}, \quad (41)\end{aligned}$$

where

$$g_W^{\text{marg}}(\mathbf{x}) = \int g_W(\mathbf{P}, \mathbf{x})\, d\mathbf{P}.$$

The particle state measured is thus represented by the function $g_W^{\text{marg}}(\mathbf{x})\delta(\mathbf{P} - \mathbf{P}_a)$, which satisfies the property required from a classical probability density, and if $\epsilon_W(\mathbf{P}, \mathbf{x})$ is itself of a classical type, we have a classical-type situation, even if for instance the function g_W is far from being of a classical type by itself.

As a usual simple case, we assume the particle state is a pure one, corresponding to a wavefunction $\varphi(\mathbf{p})$ vanishing outside a sphere of diameter D and center $\mathbf{P}_a$. The function g_W is just the opposite of a classical-type function.

2. *Classical Limit of the Invariant Density or Efficiency Functions*

The same kind of results will be obtained in this section for the invariant functions under some new hypotheses.

We will consider a sequence of invariant functions with a "space deviation" $A_x(\mathbf{P})$:

$$\bar{\zeta}(\mathbf{P}, \mathbf{u}) = \chi_{A_x}(\mathbf{P}, \mathbf{u}) \exp\,[-A_x(\mathbf{P})^2\mathbf{u}^2],$$
$$A_x(\mathbf{P}) = A_{x,0}(1 - \mathbf{v}^2)^{-\frac{1}{2}}. \quad (42)$$

The sequence is such that $1/mA_{x,0}$ goes to zero and the set $\{\chi_{A_x}\}$ is, for instance, a set of uniformly bounded functions.

A first result concerns the quantities j_I and j_F. Once smeared out in the variable P_0 with test functions slowly varying in intervals of the order of $(1/A_x) \times (1/mA_{x,0})$, they are equal to a good approximation; i.e.,

$$\int [j_I(P, x) - j_F(P, x)]\varphi(P_0)\, dP_0 = \mathcal{O}\left(\frac{P}{(mA_x)^2} \sup |\nabla_p \chi|, \frac{P_0}{(P_0A_x)^2} \sup |\varphi'_{P_0}|\right). \quad (43)$$

The physical meaning is that j_I and j_F are equivalent under most usual phenomenological situations.

If we are now interested in the functions g_F, ϵ_F [associated with kernels of the form of Eq. (42)], the results obtained in Sec. III.C.1 using g_W, ϵ_W are valid using g_F, ϵ_F with a good approximation. In fact, along similar lines as in Sec. III.B.2, g_F and g_W (respectively, ϵ_F and ϵ_W) can be shown to be equivalent to a good approximation.

A classical-type invariant function is thus characterized in the following way: it is slowly varying in phase-space regions, the dimensions of which are large compared to unity, and furthermore with a space diameter large compared to $1/m$.

In the same way, if we consider a measurement process and if the particle measured has its state defined by a density matrix of the form of Eq. (42) with $A_{x,0}$ large compared to $1/m$, we obtain, here too, a formally classical-type situation.

Classical-type situations are easily deduced along the same lines as in Sec. III.C.1.

IV. SINGLE SCATTERING

We begin the comparison of S-matrix results and classical formulas by the simplest case of a single scattering $A + B \to A_1 + B_1$.

The states of particles A, B are defined through the density matrices $\zeta_a(\mathbf{p}, \mathbf{p}')$, $\zeta_b(\mathbf{q}, \mathbf{q}')$, the final states of particles A_1, B_1 through the efficiency matrices $F_a(\mathbf{p}_1, \mathbf{p}_1')$, $F_b(\mathbf{q}_1, \mathbf{q}_1')$.

The transition probability is

$$W = \int \zeta_a^*(\mathbf{p}, \mathbf{p}')\zeta_b^*(\mathbf{q}, \mathbf{q}')F_a(\mathbf{p}_1, \mathbf{p}_1')F_b(\mathbf{q}_1, \mathbf{q}_1') \times T^*(\mathbf{p}', \mathbf{q}', \mathbf{p}_1', \mathbf{q}_1')T(\mathbf{p}, \mathbf{q}, \mathbf{p}_1, \mathbf{q}_1) \times \frac{d\mathbf{p}}{2p_0}\frac{d\mathbf{p}'}{2p_0'}\frac{d\mathbf{q}}{2q_0}\frac{d\mathbf{q}'}{2q_0'}\frac{d\mathbf{p}_1}{2p_{10}}\frac{d\mathbf{p}_1'}{2p_{10}'}\frac{d\mathbf{q}_1}{2q_{10}}\frac{d\mathbf{q}_1'}{2q_{10}'}, \quad (44)$$

where the T-matrix elements can be written as

$$T(\mathbf{p}, \mathbf{q}, \mathbf{p}_1, \mathbf{q}_1) = t(\mathbf{p}, \mathbf{q}, \mathbf{p}_1, \mathbf{q}_1)\delta(p + q - p_1 - q_1).$$

The following hypotheses, which could be weakened, are made. On one hand, the t-matrix elements will be assumed to be C^2 functions, bounded as well as their first two derivatives. On the other hand, the density and efficiency matrices will have the form given in Eq. (42). They are also such that the velocities cannot be equal all together.

We also generally assume—although it is not necessary in all cases—that the kernels $\zeta(\mathbf{p}, \mathbf{p}') = \bar{\zeta}(\mathbf{P}, \mathbf{u})$ or $F(\mathbf{p}_1, \mathbf{p}_1') = \bar{F}(\mathbf{P}_1, \mathbf{u}_1)$ (for all initial and final particles) are C^∞ functions in all variables. The C^∞ character in $\mathbf{P}$ corresponds to the usual smoothness of the Wigner functions. The C^∞ character in $\mathbf{u}$ corresponds to a rapid decrease in space of the Wigner functions.

We now use the results of Eq. (35) and the following development of the product $t(\mathbf{p}, \mathbf{q}, \mathbf{p}_1, \mathbf{q}_1)t^*(\mathbf{p}', \mathbf{q}', \mathbf{p}_1', \mathbf{q}_1')$ to the first order in the variables $\mathbf{p} - \mathbf{p}'$, $\mathbf{q} - \mathbf{q}'$, $\mathbf{p}_1 - \mathbf{p}_1'$, $\mathbf{q}_1 - \mathbf{q}_1'$:

$$t^*(\mathbf{P} - \tfrac{1}{2}\mathbf{u}, \mathbf{Q} - \tfrac{1}{2}\mathbf{v}, \mathbf{P}_1 - \tfrac{1}{2}\mathbf{u}_1, \mathbf{Q}_1 - \tfrac{1}{2}\mathbf{v}_1) \times t(\mathbf{P} + \tfrac{1}{2}\mathbf{u}, \mathbf{Q} + \tfrac{1}{2}\mathbf{v}, \mathbf{P}_1 + \tfrac{1}{2}\mathbf{u}_1, \mathbf{Q}_1 + \tfrac{1}{2}\mathbf{v}_1) = |t(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{Q}_1)|^2 \times \exp(i\mathbf{u} \cdot \nabla_P\theta + \mathbf{v}\nabla_Q\theta + \mathbf{u}_1\nabla_{P_1}\theta + \mathbf{v}_1\nabla_{Q_1}\theta) + \text{second order}, \quad (45)$$

where $\mathbf{P} = \frac{1}{2}(\mathbf{p} + \mathbf{p}')$, $\mathbf{u} = \mathbf{p} - \mathbf{p}', \cdots$, and where θ is the phase of t.

It is interesting to note that the derivative of the modulus $|t|$ does not appear in this first-order development.

A. Coarse-Grained-Type Formula

By keeping only the first-order term, we obtain the following approximation of the transition probability—we do not specify the order of error[14]:

$$W \approx \int \hat{j}_I^{(a)}\left(P, \mathbf{x} - \frac{\mathbf{P}}{P_0}x_0 + \nabla_P\theta\right) \times \hat{j}_I^{(b)}\left(Q, \mathbf{x} - \frac{\mathbf{Q}}{Q_0}x_0 + \nabla_Q\theta\right) \times \hat{E}_I^{(a)}\left(P_1, \mathbf{x} - \frac{\mathbf{P}_1}{P_{10}}x_0 + \nabla_{P_1}\theta\right) \times \hat{E}_I^{(b)}\left(Q_1, \mathbf{x} - \frac{\mathbf{Q}_1}{Q_{10}}x_0 + \nabla_{Q_1}\theta\right) \times (2\pi)^{-4}|t(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{Q}_1)|^2 \times \delta(P + Q - P_1 - Q_1)\,dP\,dQ\,dP_1\,dQ_1\,dx. \quad (46)$$

In this expression, the quantities j_I, E_I can be replaced by the corresponding quantities j_F, E_F at the limit of small $(mA_{x,0})^{-1}$ (for all particles).

It gives the following approximation:

$$W \approx \int g_F^{(a)}\left(\mathbf{P}, \mathbf{x} - \frac{\mathbf{P}}{P_0}x_0 + \nabla_P\theta\right) \times g_F^{(b)}\left(\mathbf{Q}, \mathbf{x} - \frac{\mathbf{Q}}{Q_0}x_0 + \nabla_Q\theta\right) \times \epsilon_F^{(a)}\left(\mathbf{P}_1, \mathbf{x} - \frac{\mathbf{P}_1}{P_{10}}x_0 + \nabla_{P_1}\theta\right) \times \epsilon_F^{(b)}\left(\mathbf{Q}_1, \mathbf{x} - \frac{\mathbf{Q}_1}{Q_{10}}x_0 + \nabla_{Q_1}\theta\right) \times (2\pi)^{-4}|t(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{Q}_1)|^2 \times \delta(P + Q - P_1 - Q_1)\frac{d\mathbf{P}}{2P_0}\frac{d\mathbf{Q}}{2Q_0}\frac{d\mathbf{P}_1}{2P_{10}}\frac{d\mathbf{Q}_1}{2Q_{10}}d^4x, \quad (47)$$

where $P_0 = (\mathbf{P}^2 + m^2)^{\frac{1}{2}}$, etc.

In formula (47) we note that we do not have in the integrand a product of the functions j, E at the same point x, but that each one appears with some displacement.

[14] M. Froissart, M. L. Goldberger, K. M. Watson, Phys. Rev. **131**, 2820 (1963).

As a matter of fact, there are three relative space–time displacements τ_{ba}, τ_{a_1a}, τ_{b_1a}, satisfying

$$\begin{aligned}
\boldsymbol{\tau}_{ba} - \frac{\mathbf{Q}}{Q_0}\tau_{0,ba} &= \boldsymbol{\nabla}_Q\theta - \boldsymbol{\nabla}_P\theta,\\
\boldsymbol{\tau}_{a_1a} - \frac{\mathbf{P}_1}{P_{10}}\tau_{0,a_1a} &= \boldsymbol{\nabla}_{P_1}\boldsymbol{\theta} - \boldsymbol{\nabla}_P\boldsymbol{\theta},\\
\boldsymbol{\tau}_{b_1a} - \frac{\mathbf{Q}_1}{Q_{10}}\tau_{0,b_1a} &= \boldsymbol{\nabla}_{Q_1}\boldsymbol{\theta} - \boldsymbol{\nabla}_P\boldsymbol{\theta}.
\end{aligned} \tag{48}$$

In the usual case, when the t-matrix elements are functions of two invariants only, there are only two independent scalar parameters.

The interaction is coarsely localized in some "space–time grain," the dimensions of which are given by considering the quantities τ.

B. Local-Type Scattering

If the dimension of the grains is negligible compared to the "space deviations" A_x of the particles involved, we get the following local-type formula:

$$\begin{aligned}
W \approx \int & j_F^{(a)}(P, x) j_F^{(b)}(Q, x) E_F^{(a)}(P_1, x) E_F^{(b)}(Q_1, x)\\
&\times (2\pi)^{-4} |t(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{Q}_1)|^2\\
&\times \delta(P + Q - P_1 - Q_1)\, dP\, dQ\, dP_1\, dQ_1\, d^4x.
\end{aligned} \tag{49}$$

The product of the functions j, E appears now at the same point x.

The approximation is valid if the t-matrix elements are slowly varying in intervals of the order of A_x^{-1}. The error is of the order of $(mA_{x,0})^{-1}$, so that

$$\sup_{\mathbf{R}=\mathbf{P},\mathbf{Q},\mathbf{P}_1,\mathbf{Q}_1} \left| \frac{\boldsymbol{\nabla}_{\mathbf{R}}\mathbf{t}(1 - \mathbf{V}_R^2)^{\frac{1}{2}}}{tA_{x,0}} \right|.$$

In order to compare S-matrix and classical formulas, we are first going to write down the usual phenomenological formula for classical local scattering.

1. Classical Formula for Local Scattering

The usual formula used by the experimentalists is as follows: if we define particles A, B by the probability densities $j_a(P, x)$, $j_b(Q, x)$ and the measurement apparatus of particles A_1, B_1 by the efficiencies $E_a(P_1, x)$, $E_b(Q_1, x)$, assuming furthermore the locality of the interaction, the phenomenological energy–momentum conservation and considering a phenomenological probability function $w(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{Q}_1)$, we get:

$$\begin{aligned}
W = \int & j^{(a)}(p, x) j^{(b)}(Q, x) E^{(a)}(P_1, x) E^{(b)}(Q_1, x)\\
&\times w(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{Q}_1)\\
&\times (\delta P + Q - P_1 - Q_1)\, dP\, dQ\, dP_1\, dQ_1\, dx.
\end{aligned} \tag{50}$$

We have not developed here a complete classical formalism. The phenomenological formula written here is valid for functions g and ϵ smooth enough and with sufficiently slow variation. These conditions are usually satisfied when the classical description is good.

The effective cross section is

$$\begin{aligned}
\sigma_E(\mathbf{P}, \mathbf{Q}, x) &= [\tfrac{1}{4}(PQ)^2 - (m_a m_b)^2]^{-\frac{1}{2}}\\
&\times \int E^{(a)}(P_1, x) E^{(b)}(Q_1, x) w(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{Q}_1)\\
&\times \delta(P + Q - P_1 - Q_1)\, dP_1\, dQ_1 \Big|_{\substack{P_0=(\mathbf{P}^2+m_a^2)^{\frac{1}{2}}\\ Q_0=(\mathbf{Q}^2+m_b)^{\frac{1}{2}}}}.
\end{aligned} \tag{51}$$

By using the effective cross section, the formula for the transition probability is, in fact,

$$\begin{aligned}
W = \int & j_0^{(a)}(P, x) j_0^{(b)}(Q, x) \frac{[(PQ)^2 - (m_a m_b)^2]^{\frac{1}{2}}}{P_0 Q_0}\\
&\times \sigma_E(\mathbf{P}, \mathbf{Q}, x)\, dP\, dQ\, dx.
\end{aligned} \tag{52}$$

This formula is a sophisticated expression of the usual rule $W = n_1 n_2 v\sigma$. If $\mathbf{Q} = \mathbf{0}$, then

$$\frac{[(PQ)^2 - (m_a m_b)^2]^{\frac{1}{2}}}{P_0 Q_0} = \frac{|\mathbf{P}|}{P_0} = v.$$

2. S-Matrix and Classical-Type Formulas

Equation (47) is already formally of a classical type, as is easily seen by comparing it to Eq. (49).

If the density and efficiency functions involved are themselves of a classical type, the functions $(2\pi)^{-3} j_F^{(a)}$, $(2\pi)^{-3} j_F^{(b)}$ can be replaced by functions having the properties of classical probability densities, and $E_F^{(a)}$, $E_F^{(b)}$ by functions having the properties of classical measurement efficiencies.

Adopting, furthermore, the correspondence

$$w(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{Q}_1) = (2\pi)^2 |t(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{Q}_1)|^2, \tag{53}$$

we obtain a classical-type formula for the transition probability.

Other classical-type situations can be exhibited.

In the same line of thought as in Sec. III.C.1 for studying measurement processes, we give an example here of such a situation.

In the same way as in the classical case let us define

$$\begin{aligned}
\sigma_F(\mathbf{P}, \mathbf{Q}, x) &= [\tfrac{1}{4}((PQ)^2 - (m_a m_b)^2)^{-\frac{1}{2}}\\
&\times \int E_F^{(a)}(P_1, x) E_F^{(b)}(Q_1, x) (2\pi)^2 |t(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{Q}_1)|^2\\
&\times \delta(P + Q - P_1 - Q_1)\, dP_1\, dQ_1 \Big|_{\substack{P_0=(\mathbf{P}^2+m_{a_2}^2)^{\frac{1}{2}}\\ Q_0=(\mathbf{Q}^2+m_b)^{\frac{1}{2}}}},
\end{aligned}$$

which yields

$$W \approx \int g_F^{(a)}\left(\mathbf{P}, \mathbf{x} - \frac{\mathbf{P}}{P_0} x_0\right) \times g_F^{(b)}\left(\mathbf{Q}, \mathbf{x} - \frac{\mathbf{Q}}{Q_0} x_0\right) \sigma_F(\mathbf{P}, \mathbf{Q}, x) \times 4[(PQ)^2 - (m_a m_b)^2]^{\frac{1}{2}} \frac{d\mathbf{P}}{2P_0} \frac{d\mathbf{Q}}{2Q_0} d^4x. \quad (54)$$

If we assume that $g_F^{(a)}$ and $g_F^{(b)}$ are negligible outside spheres of diameter D and centers $\mathbf{P}_a$, $\mathbf{Q}_b$ in the variables $\mathbf{P}$, $\mathbf{Q}$ and that $[(PQ)^2 - (m_a m_b)^2]^{\frac{1}{2}}\sigma_F$ is slowly varying in $\mathbf{P}$, $\mathbf{Q}$ in an interval of the order of D, it is possible to obtain the following approximation:

$$W \approx \int j_{\text{marg}}^{(a)}(x) j_{\text{marg}}^{(b)}(x) \hat{\sigma}_{\mathbf{P_a}, \mathbf{Q_b}}(x)\, d^4x, \quad (55)$$

where

$$j_{\text{marg}}^{(a)}(x) = \int g_F^{(a)}\left(\mathbf{P}, \mathbf{x} - \frac{\mathbf{P}}{P_0} x_0\right) \frac{d\mathbf{P}}{2P_0},$$

$$j_{\text{marg}}^{(b)}(x) = \int g_F^{(b)}\left(\mathbf{Q}, \mathbf{x} - \frac{\mathbf{Q}}{Q_0} x_0\right) \frac{d\mathbf{Q}}{2Q_0},$$

$$\hat{\sigma}_{P_a, Q_b}(x) = \{4[(P, Q)^2 - (m_a, m_b)^2]^{\frac{1}{2}}\sigma_F(\mathbf{P}, \mathbf{Q}, x)\}_{\substack{\mathbf{P}=\mathbf{P_a} \\ \mathbf{Q}=\mathbf{Q_b}}}.$$

We also assume that the kernels of the density matrices are C^∞ functions of the form of Eq. (42). The C^∞ character implies that the functions g_F are rapidly decreasing as functions of $\mathbf{y}_P = \mathbf{x} - (\mathbf{P}/P_0)x_0$, $\mathbf{y}_Q = \mathbf{x} - (\mathbf{Q}/Q_0)x_0$. If they are assumed to be negligible outside spheres of dimension d and if the velocities of the two particles cannot be equal [$|(\mathbf{P}/P_0) - (\mathbf{Q}/Q_0)|$ is of the order of one], the product $g_F^{(a)}(\mathbf{p}, \mathbf{y}_P) g_F^{(b)}(\mathbf{Q}, \mathbf{y}_Q)$ is then negligible outside a sphere of dimension d in all directions of space-time, in particular for $|x_0|$ larger than d.

Assuming a condition of the type

$$\frac{dD}{P_0 A_x}\left(\text{resp } \frac{dD}{Q_0 A_x}\right) \ll 1,$$

we obtain the approximation

$$W \approx \int g_{\text{marg}}^{(a)}\left(\mathbf{x} - \frac{\mathbf{P}}{P_0} x_0\right) \delta(\mathbf{P} - \mathbf{P_a}) \times g_{\text{marg}}^{(b)}\left(\mathbf{x} - \frac{\mathbf{Q}}{Q_0} x_0\right) \delta(\mathbf{Q} - \mathbf{Q_a}) \times \hat{\sigma}(\mathbf{P}, \mathbf{Q}, x)\, d^4x\, d\mathbf{P}\, d\mathbf{Q}, \quad (56)$$

where

$$g_{\text{marg}}^{(a)}\left(\mathbf{x} - \frac{\mathbf{P_a}}{P_{a,0}} x_0\right) = \int g_F^{(a)}\left(\mathbf{P}, \mathbf{x} - \frac{\mathbf{P_a}}{P_{a,0}} x_0\right) \frac{d\mathbf{P}}{2P_0},$$

$$g_{\text{marg}}^{(b)}\left(\mathbf{x} - \frac{\mathbf{Q_b}}{Q_{b,0}} x_0\right) = \int g_F^{(b)}\left(\mathbf{Q}, \mathbf{x} - \frac{\mathbf{Q_b}}{Q_{b,0}} x_0\right) \frac{d\mathbf{Q}}{2Q_0}.$$

The functions $g_{\text{marg}}^{(a)}$, $g_{\text{marg}}^{(b)}$ can be replaced by positive functions at the approximation $(mA_{x,0})^{-1} \ll 1$.

Thus if, for instance, the efficiency functions are of a classical type, we obtain here too a classical-type formula, even for density functions which are far from being themselves of a classical type.

The same comments can be made as in the case of the measurement processes studied in Sec. III.C.1.

C. Other Possible Situations

We end this part with the following remark: We have studied until now S-matrix results under special conditions of slow variation of the t-matrix elements, which allowed us to obtain coarse-grained-type or local-type formulas.

If these conditions are not satisfied, we may obtain very different results. For instance, if the t-matrix elements have some polelike behavior, this situation can correspond in some cases to a physical process of creation of an intermediate propagating unstable particle in the scattering $A + B \to M$, followed by the decay of M into particles A_1, B_1.

Such a case is similar to what is studied in the next part, to which we refer.

V. MULTIPLE SCATTERING

In Sec. V, our aim is to show directly how it is possible to obtain the usual classical type formulas for different situations of multiple scattering.

In Sec. V.A a polelike behavior of the connected matrix elements is assumed in a weak form. A general formula is obtained and we show how it leads under various conditions either to the usual bump in the cross sections (e.g., N^*) or to a formula for successive scatterings with the propagation of a real intermediate stable or unstable particle (e.g., neutron) or to intermediate cases, where only a one-mass-shell kinematical condition for the "intermediate" particle is expressed (e.g., Σ^0).

In Sec. V.B, a simple case of Landau-type behavior of the connected matrix elements is exhibited as an example, and it is shown how it can correspond to a physical process of successive and multiple scatterings.

As we are interested in successive interactions which can be separated by macroscopic distances, a parameter ρ corresponding to the separation is explicitly introduced.

A. Double Scattering

Let us consider the scattering $A + B + C \to A_1 + B_1 + C_1$.

The states of particles A, B, C are defined through the density-matrix kernels $\zeta_a(\mathbf{p}, \mathbf{p}')$, $\zeta_b(\mathbf{q}, \mathbf{q}')$, $\zeta_c(\mathbf{r}, \mathbf{r}')$,

the final states of particles A_1, B_1, C_1 through the efficiency-matrix kernels $F_a(\mathbf{p}_1, \mathbf{p}_1')$, $F_b(\mathbf{q}_1, \mathbf{q}_1')$, $F_c(\mathbf{r}_1, \mathbf{r}_1')$.

The transition probability is

$$W = \int \zeta_a^*(\mathbf{p}, \mathbf{p}')\zeta_b^*(\mathbf{q}, \mathbf{q}')\zeta_c^*(\mathbf{r}, \mathbf{r}') \times F_a(\mathbf{p}_1, \mathbf{p}_1')F_b(\mathbf{q}_1, \mathbf{q}_1')F_c(\mathbf{r}_1, \mathbf{r}_1') \times T(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1)T^*(\mathbf{p}', \mathbf{q}', \mathbf{r}', \mathbf{p}_1', \mathbf{q}_1', \mathbf{r}_1') \times \pi \frac{d\mathbf{p}}{2p_0} \pi \frac{d\mathbf{p}'}{2p_0'} \pi \frac{d\mathbf{p}_1}{2p_{10}} \pi \frac{d\mathbf{p}_1'}{2p_{10}'},$$

where

$$\pi \frac{d\mathbf{p}}{2p_0} = \frac{d\mathbf{p}}{2p_0} \frac{d\mathbf{q}}{2q_0} \frac{d\mathbf{r}}{2r_0}, \quad \text{etc.}$$

The T-matrix elements can be written as

$$T(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) = t(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1)\delta(p + q + r - p_1 - q_1 - r_1).$$

Along the lines of Sec. II.D, the t-matrix elements are now written as

$$t(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) = \frac{\mathcal{M}(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1)}{k^2 - m^2 + i\gamma}, \quad (57)$$

where $k = p + q - p_1$ and where γ is zero for a stable particle.

The $\mathcal{M}$-matrix elements are assumed to be C^1 functions at least. Furthermore, some hypothesis about their variation is made to make formula (57) meaningful when $\gamma \neq 0$: The $\mathcal{M}$-matrix elements are assumed to be slowly varying in an interval of the order of γ/k_0 in each variable, the kinematic (and other) conditions being such that k_0 is positive and bounded below. In particular, it will be slowly varying as a function of k^2 in an interval of the order of γ (for $|\mathbf{k}/k_0|$ of the order of or smaller than unity).

If, as usually assumed, $\mathcal{M}$ is function of the invariants only, such that

$$\mathcal{M}(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) = \hat{\mathcal{M}}(k^2, \cdots),$$

it is enough to assume that the function $\hat{\mathcal{M}}$ is slowly varying in k^2 in an interval of the order of γ.

1. General Formulas

For the sake of simplicity, we do not consider coarse-grained-type formulas for each individual scattering.

Assuming that the function $\mathcal{M}$ is slowly varying over intervals of the order of A_x^{-1} in all variables—the density and efficiency functions are assumed to have "space deviations" A_x—we obtain the following approximation for the transition probability (for particles C, B, C_1 translated through a vector ρ)—with an error of the order of $|\nabla\mathcal{M}/\mathcal{M}A_x|$:

$$W(\rho) \approx \int \zeta_a^*(\mathbf{p}, \mathbf{p}')\zeta_b^*(\mathbf{q}, \mathbf{q}')\zeta_c^*(\mathbf{r}, \mathbf{r}') \times F_a(\mathbf{p}_1, \mathbf{p}_1')F_b(\mathbf{q}_1, \mathbf{q}_1')F_c(\mathbf{r}_1, \mathbf{r}_1') \times \delta\left(\frac{p + p'}{2} - P\right)\delta\left(\frac{q + q'}{2} - Q\right) \times \delta\left(\frac{r + r'}{2} - R\right)\delta\left(\frac{p_1 + p_1'}{2} - P_1\right) \times \delta\left(\frac{q_1 + q_1'}{2} - Q_1\right)\delta\left(\frac{r_1 + r_1'}{2} - R_1\right) \times \delta(p - p' + q - q_1' - (p_1 - p_1')) - l) \times \delta(l + r - r' - (q_1 - q_1')) - (r_1 - r_1')) \times \pi \frac{d\mathbf{p}}{2p_0} \pi \frac{d\mathbf{p}'}{2p_0'} \pi \frac{d\mathbf{p}_1}{2p_{10}} \pi \frac{d\mathbf{p}_1'}{2p_{10}'} \times |\mathcal{M}(\mathbf{P}, \mathbf{Q}, \mathbf{R}, \mathbf{P}_1, \mathbf{Q}_1, \mathbf{R}_1)|^2 \times \delta(P + Q - P_1 - K)\delta(K + R - Q_1 - R_1) \times dP\, dQ\, dR\, dP_1\, dQ_1\, dR_1 \times \frac{1}{(K + l/2)^2 - m^2 + i\gamma} \times \frac{1}{(K - l/2)^2 - m^2 - i\gamma} \exp(-il\rho)\, dK\, dl. \quad (58)$$

This formula may be written as follows:

$$W(\rho) \approx \int j_I^{(a)}(P, x)j_I^{(b)}(Q, x) \times E_I^{(a)}(P_1, x)E_I^{(b)}(Q_1, y)E_I^{(c)}(R_1, y)j_I^{(c)}(R, y) \times (2\pi)^{-8} |\mathcal{M}(\mathbf{P}, \mathbf{Q}, \mathbf{R}, \mathbf{P}_1, \mathbf{Q}_1, \mathbf{R}_1)|^2 \times \delta(P + Q - P_1 - K)\delta(K + R - Q_1 - R_1) \times \mathfrak{D}(K, y - x + \rho) \times dP\, dQ\, dR\, dP_1\, dQ_1\, dR_1\, dK\, dx\, dy. \quad (59)$$

A "generalized propagator" $\mathfrak{D}(K, x)$ has been introduced, such that

$$\mathfrak{D}(K, x) = \int \exp(-ilx) \frac{1}{(K + l/2)^2 - m^2 + i\gamma} \times \frac{1}{(K - l/2)^2 - m^2 - i\gamma} dl. \quad (60)$$

It may be written by using the causal Green's function as:

$$\mathfrak{D}(K, x) = [D^c(2x) \exp(-2iKx)] * [D^c(-2x) \exp(2iKx)],$$

$$D^c(x) = -(2\pi)^{-4} \int \exp(ikx)(k^2 - m^2 + i\gamma)^{-1}\, dk.$$

However, we are not interested in this general case and we do consider the usual conditions, when $A_{x,0}$ is large compared to the inverse of all the masses of the particles involved. This allows one to replace the functions j_I, E_I by the functions j_F, E_F.

Furthermore, a new important approximation is as follows. For convenience, we write Eq. (58) in the form

$$W \approx \int F(K, l) \frac{1}{K^2 + l^2/4 + m^2 + Kl + i\gamma} \times \frac{1}{K^2 + l^2/4 - m^2 - Kl - i\gamma} dK\, dl, \quad (61)$$

where the function F is obtained by integrating the right-hand side of Eq. (58) on all variables except K, l.

For kernels of density and efficiency matrices of the form of Eq. (43), the function $F(K, l)$ is thus slowly varying in $K(\mathbf{K}, K_0)$ over intervals of the order of A_p and is, on the contrary, exponentially decreasing in the variable $l(\mathbf{l}, l_0)$, i.e., it is negligible for $|l_0|$, $|\mathbf{l}|$ large compared to A_x^{-1}.

Owing to that behavior, we can show that it is possible, to a good approximation, to replace $K^2 + l^2/4$ in both propagators by K^2. In fact, let us consider the following quantities:

$$W = \int F(K, l) \frac{1}{K^2 + l^2/4 - m^2 + Kl + i\gamma} \times \frac{1}{K^2 + l^2/4 - m^2 - Kl - i\gamma} dK\, dl,$$

$$W' = \int F(K, l) \frac{1}{K^2 - m^2 + Kl + i\gamma} \times \frac{1}{K^2 - m^2 - Kl - i\gamma} dK\, dl.$$

Defining

$$F_1(K, l) = \frac{F(K, l)}{2(K_0^2 - l_0^2)} = \hat{F}_1(K^2 + l^2/4 - m^2, \mathbf{K}, Kl, \mathbf{l}),$$

$$F_2(K, l) = \frac{F(K, l)}{2K_0^2} = \hat{F}_2(K^2 - m^2, \mathbf{K}, Kl, \mathbf{l}),$$

we get

$$W - W' = \int [\hat{F}_1(s, \mathbf{K}, t, \mathbf{l}) - \hat{F}_2(s, \mathbf{K}, t, \mathbf{l})] \times \frac{1}{s + t + i\gamma} \frac{1}{s - t - i\gamma} ds\, d\mathbf{K}\, dt\, d\mathbf{l}.$$

From the result, it can be actually shown that $W - W'$ is negligible with $(K_0 A_x)^{-1}$.

In that way we obtain a new approximation for $W(\rho)$, where the function $\mathfrak{D}(K, x)$ in Eq. (59) is replaced by

$$\hat{\mathfrak{D}}(K, x) = \int \exp(ilx) \frac{1}{K^2 - m^2 + Kl + i\gamma} \times \frac{1}{K^2 - m^2 - Kl - i\gamma} dl. \quad (62)$$

A straightforward calculation gives (for $K_0 > 0$):

$$\hat{\mathfrak{D}}(K, x) = \frac{(2\pi)^4}{K_0} \delta\left(\mathbf{x} - \frac{\mathbf{K}}{K_0} x_0\right) \theta(x_0) \exp\left(-\frac{\gamma x_0}{K_0}\right) \times \int_{-x_0/2K_0}^{x_0/2K_0} \exp(i(K^2 - m^2)u)\, du. \quad (63)$$

The final formula we get is thus

$$W(\rho) \approx \int j_F^{(a)}(P, x) j_F^{(b)}(Q, x) \times E_F^{(a)}(P_1, x) j_F^{(c)}(R_1, y) E_F^{(b)}(Q_1, y) E_F^{(c)}(R_1, y) \times \frac{(2\pi)^{-8}}{K_0} |\mathcal{M}(\mathbf{P}, \mathbf{Q}, \mathbf{R}, \mathbf{P}_1, \mathbf{Q}_1, \mathbf{R}_1)|^2 \cdot \times \delta(P + Q - P_1 - K) \delta(K + R - Q_1 - R_1) \times \hat{\mathfrak{D}}(K, y - x + \rho) \times dP\, dQ\, dR\, dP_1\, dQ_1\, dR_1\, dK\, dx\, dy. \quad (64)$$

The function $\hat{\mathfrak{D}}$ already contains the factor

$$\theta(x_0) \delta\left(\mathbf{x} - \frac{\mathbf{K}}{K_0} x_0\right) \exp\left(-\frac{\gamma x_0}{K_0}\right),$$

which has formally the form of a classical factor corresponding to the propagation of an unstable (or stable for $\gamma = 0$) particle after its creation [the factor $\theta(x_0)$ accounting thus for causality]. However, the mass-shell condition does not obtain in general.

We are now going to show how Eq. (64) leads to the usual classical-type formulas.

2. *Observation of a Resonance*

Let us now assume the following condition:

$$\frac{\gamma}{K_0} \gg \frac{1}{A_x}. \quad (65)$$

Because of the presence of the damping exponential $\exp(-\gamma z_0/K_0)$ in Eq. (64), the main contribution to the integrand is obtained for $|z_0| \ll A_x$ (where $z = y - x + \rho$). A similar condition holds for $|\mathbf{z}|$ due to the factor $\delta(\mathbf{z} - (\mathbf{K}/K_0) z_0)$.

We thus limit ourselves to the case $\rho = 0$ as there is no point in considering large values of ρ.

Looking at Eq. (58), it is now possible to neglect Kl as compared to γ in both denominators $K^2 - m^2 + Kl + i\gamma$, $K^2 - m^2 - Kl - i\gamma$ and to obtain, with an

error of the order of $K_0/(\gamma A_x)$, the following approximation:

$$W \approx \int j_F^{(a)}(P, x) j_F^{(b)}(Q, x) j_F^{(c)}(R, x) \times E_F^{(a)}(P_1, x) E_F^{(b)}(Q_1, x) E_F^{(c)}(R_1, x) \times \frac{(2\pi)^4}{K_0} \delta(P + Q - P_1 - K) \times \delta(K + R - Q_1 - R_1) \times \frac{|\mathcal{M}(\mathbf{P}, \mathbf{Q}, \mathbf{R}, \mathbf{P}_1, \mathbf{Q}_1, \mathbf{R}_1)|^2}{(K^2 - m^2)^2 + \gamma^2} \times dP\, dQ\, dR\, dP_1\, dQ_1\, dR_1\, dK\, dx, \quad (66)$$

where we recall that $\mathcal{M}$ is slowly varying in K^2 in an interval of the order of γ.

In that special case, it would be more suitable to obtain this formula directly from Eq. (58).

It is formally a classical-type formula for a local scattering with a bump in the cross sections. As a matter of fact, it is difficult to have an interaction between three joined particles and the corresponding formula is more usual for the case of two initial interacting particles.

3. *On Mass-Shell Kinematical Condition for the "Intermediate" Particle*

A particularly interesting case is usual and corresponds to the condition stronger than condition (65), so that

$$A_x^{-1} \ll \gamma/K_0 \ll A_p. \quad (67)$$

If we consider Eq. (66) in the limit when γ/K_0 is small compared to A_p, it is possible to replace the factor

$$\frac{1}{\gamma} \frac{\gamma}{(K^2 - m^2)^2 + \gamma^2} \quad \text{by} \quad \frac{1}{\gamma} \delta(K^2 - m^2).$$

In fact, in this case, it is phenomenologically neither possible to see a bump corresponding to a resonance nor to see an intermediate propagating particle, but only to observe the on-mass-shell kinematical condition $(P + Q - P_1)^2 = m^2$.

Here too, the case of two initial particles is more usual. Experimentally, if one still wants to speak of an "intermediate" particle with a lifetime τ or a resonance width, one can only deduce that the following inequality holds:

$$A_x^{-1} \ll \gamma/K_0 \ll A_p.$$

It is the case for the measurement of the Σ_0 lifetime:

$$10^{11}\ \text{sec}^{-1} < \tau_{\Sigma_0}^{-1} < 10^{22}\ \text{sec}^{-1}.$$

4. *Propagation of an Intermediate Real Particle*

We aim in that section to study the case of a classical-type formula corresponding to an actual propagation of a real intermediate particle between two successive scatterings.

Particle C will then be assumed to be away from particles A, B at time zero. In practice, the following conditions will hold. The density and efficiency matrix kernels will be C^∞ functions. As already stated in Sec. IV.B, the product $g_F^{(a)}(\mathbf{P}, \mathbf{x} - (\mathbf{P}/P_0)x_0) g_F^{(b)}(\mathbf{Q}, \mathbf{x} - (\mathbf{Q}/Q_0)x_0)$ is then rapidly decreasing in all space–time directions, for different velocities of A and B. If it is assumed to be negligible for $|\mathbf{x}|$, $|x_0|$ larger than some quantity d ($d \geq A_x$), the first interaction is then localized in this region.

The product

$$g_F^{(c)}\left(\mathbf{R}, \mathbf{y} - \frac{\mathbf{R}}{R_0} y_0\right) E_F^{(b)}\left(\mathbf{Q}_1, \mathbf{y} - \frac{\mathbf{Q}_1}{Q_{10}} y_0\right) \times E_F^{(c)}\left(\mathbf{R}_1, \mathbf{y} - \frac{\mathbf{R}_1}{R_{10}} y_0\right)$$

is also assumed to be negligible for $|\mathbf{y}|$, $|y_0|$ larger than d.

To say that particle C is away from A and B at time zero means that $|\rho_0|$ will be taken large compared to d. Owing to the damping exponential factor $\exp(-\gamma z_0/K_0)$ ($z = y - x + \rho$, $|z_0| \sim |\rho_0|$), we have to assume, similarly, in order to obtain a non-negligible transition probability, that

$$(\gamma/K_0)\,|\rho_0| \lesssim 1, \quad \gamma/K_0 \ll 1/A_x. \quad (68)$$

Condition (68) is just opposite to the condition expressed in Sec. V.A.2.

We also note, as expected, that the transition probability is rapidly decreasing with ρ_0, for ρ_0 negative, and is negligible for $-\rho_0$ larger than d, due to the causality factor $\theta(z_0)$ in formula (64).

Assuming $\rho_0 > 0$ and condition (68), we consider in the right-hand side of Eq. (64) the factor

$$\int_{-z_0/2K_0}^{z_0/2K_0} \exp\,[i(K^2 - m^2)u]\, du,$$

where

$$z_0 = y_0 - x_0 + \rho_0, \quad z_0 > 0.$$

For ρ_0 large compared to d, it is possible to use the following approximation:

$$\int_{-z_0/2K_0}^{z_0/2K_0} \exp\,[i(K^2 - m^2)u]\, du \sim 2\pi\delta(K^2 - m^2), \quad (69)$$

which can be justified because of the smoothness with respect to momentum variables of all the functions involved in Eq. (64).

The following formula is obtained:

$$
\begin{aligned}
W \approx \int & j_F^{(a)}(P, x) j_F^{(b)}(Q, x) \\
& \times E_F^{(a)}(P_1, x) j_F^{(c)}(R, y) E_F^{(b)}(Q_1, y) E_F^{(c)}(R_1, y) \\
& \times \delta\left(\mathbf{y} - \mathbf{x} + \boldsymbol{\rho} - \frac{\mathbf{K}}{K_0}(y_0 - x_0 + \rho_0)\right) \\
& \times \theta(y_0 - x_0 + \rho_0) \exp\left[-\frac{\gamma(y_0 - x_0 + \rho_0)}{K_0}\right] \\
& \times |\mathcal{M}(\mathbf{P}, \mathbf{Q}, \mathbf{R}, \mathbf{P}_1, \mathbf{Q}_1, \mathbf{R}_1)|^2 \\
& \times \delta(P + Q - P_1 - K)\delta(K + R - Q_1 - R_1) \\
& \times \frac{(2\pi)^3}{2K_0}\delta(K^2 - m^2)\theta(K_0) \\
& \times dP\, dQ\, dR\, dP_1\, dQ_1\, dR_1\, dx\, dy\, dK. \qquad (70)
\end{aligned}
$$

For the case when $\gamma = 0$, the usual factorization property of $\mathcal{M}$ is assumed:

$$
\begin{aligned}
\mathcal{M}(\mathbf{P}, \mathbf{Q}, \mathbf{R}, \mathbf{P}_1, \mathbf{Q}_1, \mathbf{R}_1)\big|_{K_0 = (\mathbf{K}^2 + m^2)^{\frac{1}{2}}} \\
= \frac{1}{2\pi} t(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{K}) t(\mathbf{K}, \mathbf{R}, \mathbf{Q}_1, \mathbf{R}_1). \qquad (71)
\end{aligned}
$$

For the case of an unstable particle, it is still assumed that, at least with a good approximation, a factorization property also holds:

$$
\begin{aligned}
\mathcal{M}(\mathbf{P}, \mathbf{Q}, \mathbf{R}, \mathbf{P}_1, \mathbf{Q}_1, \mathbf{R}_1)\big|_{K_0 = (\mathbf{K}^2 + m^2)^{\frac{1}{2}}} \\
\approx \frac{1}{2\pi} \mathcal{M}_1(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1) \mathcal{M}_2(\mathbf{R}, \mathbf{Q}_1, \mathbf{R}_1). \qquad (72)
\end{aligned}
$$

Classical formula. Along the lines of Sec. II.D, we write now the usual classical phenomenological formula corresponding to two successive scatterings.

The first scattering $A + B \to A_1 + M$ is considered and the current intensity of the intermediate particle M is written as

$$
\begin{aligned}
j_{\text{int}}(K, y) = & \frac{1}{2K_0}\delta(K^2 - m^2)\theta(K_0) \\
& \times \int j_a(P, x) j_b(Q, x) E_a(P_1, x) \\
& \times \delta[\mathbf{y} - \mathbf{x} - (\mathbf{K}/K_0)(y_0 - x_0)]\theta(y_0 - x_0) \\
& \times \exp\{-[\gamma(y_0 - x_0)]/K_0\} w_1(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{K}) \\
& \times \delta(P + Q - P_1 - K)\, dP\, dQ\, dP_1\, dx. \qquad (73)
\end{aligned}
$$

We have used the hypothesis of locality of the first interaction, and the fact that after its creation we deal with a propagating particle of mass m (which may be unstable).

We also note that the quantity

$$\int j_{\text{int}}^0(K, y)\, dK\, d\mathbf{y}$$

depends now on the time y_0. If the product

$$j_a(P, x) j_b(Q, x) E_a(P_1, x)$$

is negligible for $|\mathbf{x}|$, if $|x_0|$ is larger than some quantity d, and if y_0 is positive and large compared to d, the following approximation can be used:

$$
\begin{aligned}
& j_{\text{int}}(K, y)_{y_0 \gg d} \\
& \quad \approx \frac{1}{2K_0}\delta(K^2 - m^2)\theta(K_0) \exp\left(-\frac{\gamma y_0}{K_0}\right) \\
& \qquad \times \int j_a(P, x) j_b(Q, x) E_a(P_1, x) \\
& \qquad \times \delta(\mathbf{y} - \mathbf{x} - (\mathbf{K}/K_0)(y_0 - x_0)) w_1(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{K}) \\
& \qquad \times \delta(P + Q - P_1 - K)\, dP\, dQ\, dP_1\, dx \\
& \quad = \exp(-\gamma y_0/K_0) j'_{\text{int}}(K, y) \qquad (74a)
\end{aligned}
$$

with

$$
\begin{aligned}
& \int j'^0_{\text{int}}(K, y)\, dK\, d\mathbf{y} \\
& \quad = \int j_a(P, x) j_b(Q, x) E_a(P_1, x) \\
& \qquad \times \delta(K^2 - m^2)\theta(K_0) w_1(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{K}) \\
& \qquad \times \delta(P + Q - P_1 - K)\, dP\, dQ\, dP_1\, dx = W_1, \qquad (74b)
\end{aligned}
$$

where $\delta(K^2 - m^2)\theta(K_0)$ is the efficiency of an apparatus measuring all possible states of the particle M.

We consider now the second scattering

$$M + C \to B_1 + C_1,$$

and we obtain the transition probability of the whole process:

$$
\begin{aligned}
W(\rho) = & \int j_a(P, x) j_b(Q, x) E_a(P_1, x) \\
& \times j_c(R, y) E_b(Q_1, y) E_c(R_1, y) \\
& \times \delta[\mathbf{y} - \mathbf{x} + \boldsymbol{\rho} - (\mathbf{K}/K_0)(y_0 - x_0 + \rho_0)] \\
& \times \theta(y_0 - x_0 + \rho_0) \\
& \times \exp\{-[\gamma(y_0 - x_0 + \rho_0)]/K_0\} \\
& \times \delta(P + Q - P_1 - K)\delta(K + R - Q_1 - R_1) \\
& \times w_1(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{K}) w_2(\mathbf{K}, \mathbf{R}, \mathbf{Q}_1, \mathbf{R}_1)\delta(K^2 - m^2) \\
& \times \theta(K_0)\frac{1}{2K_0}\, dP\, dQ\, dR\, dP_1\, dQ_1\, dR_1\, dK\, dx\, dy. \\
& \qquad (75)
\end{aligned}
$$

It is easy now to see how formulas of this type are obtained in S-matrix theory. In fact, by replacing in formula (70), $(2\pi)^{-3} j_F^{(a)(b)(c)}$ by $j_{(a)(b)(c)}$, $E_F^{(a)(b)(c)}$ by $E_{(a)(b)(c)}$, $|\mathcal{M}(\mathbf{P}, \mathbf{Q}, \mathbf{R}, \mathbf{P}_1, \mathbf{Q}_1, \mathbf{R}_1)|^2$ by

$$(2\pi)^{-6} w_1(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{K}) w_2(\mathbf{K}, \mathbf{R}, \mathbf{Q}_1, \mathbf{R}_1),$$

formula (75) is (formally) obtained.

Classical-type situations can be studied along similar lines as in Sec. IV.

Special cases. If we consider $W(\rho)$, it can be written as

$$W(\rho) = \int w(\rho, \mathbf{K})\, d\mathbf{K},$$

where $w(\rho, \mathbf{K})$ is obtained by integrating over all variables except $\mathbf{K}$ in the right-hand side of Eq. (70).

We then note that $w(\rho, \mathbf{K})$ is negligible for $|\rho - (\mathbf{K}/K_0)\rho_0|$ larger than d. The kinematic conditions may determine a region for $\mathbf{K}$ outside of which $w(\rho, \mathbf{K})$ is negligible. If the quantity $|\boldsymbol{\rho} - (\mathbf{K}/K_0)\rho_0|$ is larger than d over all that region, $W(\rho)$ is still negligible.

B. Multiple Scattering

We consider now the general case of a Landau-type behavior of the t-matrix elements (in the physical region). We treat as an example the case of a scattering $A + B + C \to A_1 + B_1 + C_1$, assuming the following hypothesis on the t-matrix elements:

$$t(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) = \int \frac{\mathcal{M}(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1, k_1, k_2, k_3)}{D_1(k_1) D_2(k_2) D_3(k_3)} \times \delta(p + q - k_1 - k_2) \times \delta(p_1 + q_1 - k_1 - k_3)\, dk_1\, dk_2\, dk_3, \quad (76)$$

where $\mathcal{M}$ is a C^1 function satisfying, furthermore,

$$\mathcal{M}(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1, k_1, k_2, k_3)|_{k_1^2 = m_i^2} = (2\pi)^{-3} t(\mathbf{p}, \mathbf{q}, \mathbf{k}_1, \mathbf{k}_2) t(\mathbf{k}_1, \mathbf{k}_3, \mathbf{p}_1, \mathbf{q}_1) t(\mathbf{k}_2, \mathbf{r}, \mathbf{r}_1, \mathbf{k}_3), \quad (77)$$

and where

$$D_i(k_i) = (k_i^2 - m_i^2 + i\epsilon)^{-1}.$$

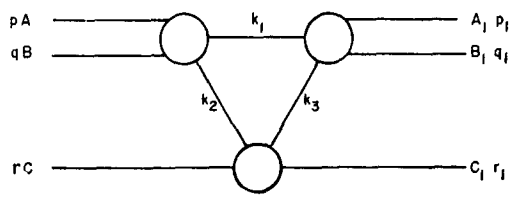

FIG. 1. The unitarity graph.

These hypotheses guarantee that t has the singularity corresponding to the unitarity graph (Fig. 1).

We note that $\mathcal{M}$ is not uniquely determined and can always be chosen with a compact support around the points $k_i^2 = m_i^2$. In fact, it is sufficient to consider any C^1 function $\hat{\mathcal{M}}$ with a compact support around these points and satisfying property (77) and a C^1 function $\varphi(k_1, k_2, k_3)$ satisfying the same condition of support and furthermore

$$\int \varphi(k_1, k_2, k_3)\delta(p + q - k_1 - k_2) \times \delta(p_1 + q_1 - k_1 - k_3)\, dk_1\, dk_2\, dk_3 = 1,$$

for p, q, p_1, q_1 defined by the kinematics. We then define

$$\mathcal{M} = \hat{\mathcal{M}} + \varphi(k_1, k_2, k_3) \prod_{i=1,2,3} (k_i^2 - m_i^2) \times \left[t - \int \frac{\hat{\mathcal{M}}}{D_1 D_2 D_3} \delta(p + q - k_1 - k_2) \times \delta(p_1 + q_1 - k_1 - k_3)\, dk_1\, dk_2\, dk_3 \right].$$

Particles C, C_1 will be taken away with a 4-vector ρ; particles A_1, B_1 with a 4-vector σ.

Using expression (76) and assuming that the function $\mathcal{M}$ can be chosen to be slowly varying in intervals of the order of A_x^{-1}, where A_x is the "space deviation" of all density and efficiency functions involved, the following approximation will hold:

$$\begin{aligned} W(\rho, \sigma) = \int & \zeta_a^*(\mathbf{p}, \mathbf{p}')\zeta_b^*(\mathbf{q}, \mathbf{q}')\zeta_c^*(\mathbf{r}, \mathbf{r}')F_a(\mathbf{p}_1, \mathbf{p}_1')F_b(\mathbf{q}_1, \mathbf{q}_1')F_c(\mathbf{r}_1, \mathbf{r}_1') \\ & \times \delta\left(\frac{p + p'}{2} - P\right)\delta\left(\frac{q + q'}{2} - Q\right)\delta\left(\frac{r + r'}{2} - R\right)\delta\left(\frac{p_1 + p_1'}{2} - P_1\right)\delta\left(\frac{q_1 + q_1'}{2} - Q_1\right)\delta\left(\frac{r_1 + r_1'}{2} - R_1\right) \\ & \times \delta(P + Q - K_1 - K_2)\delta(K_1 + K_3 - P_1 - Q_1)\delta(R + K_2 - K_3 - R_1) \\ & \times \delta(p - p' + q - q' - l_1 - l_2)\delta(l_1 + l_3 - (p_1 - p_1') - (q_1 - q_1'))\delta(r - r' + l_2 - (r_1 - r_1') - l_3) \\ & \times |\mathcal{M}(\mathbf{P}, \mathbf{Q}, \mathbf{R}, \mathbf{P}_1, \mathbf{Q}_1, \mathbf{R}_1, K_1, K_2, K_3)|^2 \prod_{i=1,2,3} D_i\left(K_i + \frac{l_i}{2}\right) D_i^*\left(K_i - \frac{l_i}{2}\right) \\ & \times \exp\{i\rho[r - r' - (r_1 - r_1')]\} \exp\{i\sigma[q_1 - q_1' + p_1 - p_1')]\} \\ & \times \pi \frac{d\mathbf{p}}{2p_0} \pi \frac{d\mathbf{p}'}{2p_0'} \pi \frac{d\mathbf{p}_1}{2p_{10}} \pi \frac{d\mathbf{p}_1'}{2p_{10}'} dP\, dQ\, dR\, dP_1\, dQ_1\, dR_1 \prod_{i=1,2,3} dK_i\, dl_i. \end{aligned} \quad (78)$$

Along the same lines as in Sec. V.A, we use

$$\delta(p - p' + q - q' - l_1 - l_2)$$
$$= (2\pi)^{-4}\int \exp\,[i(p - p' + q - q' - l_1 - l_2)x]\,dx,$$
$$\delta(l_1 + l_3 - (p_1 - p_1') - (q_1 - q_1'))$$
$$= (2\pi)^{-4}\int \exp\,\{i[l_1 + l_3 - (p_1 - p_1') - (q_1 - q_1')]y\}\,dy,$$
$$\delta(r - r' + l_2 - (r_1 - r_1') - l_3)$$
$$= (2\pi)^{-4}\int \exp\,\{i[r - r' + l_2 - (r_1 - r_1') - l_3]z\}\,dz. \tag{79}$$

The same approximations will also be used, since, by construction of $\mathcal{M}$, $|K_{0i}|$ is larger than or of the order of m_i and that negative values of K_{0i} will not contribute for large positive ρ_0, σ_0.

The parameter d may be introduced for the three bubbles (A, B), (A_1, B_1), (C, C_1) and we will then obtain for ρ_0, σ_0 large compared to d a classical-type formula corresponding to three scattering processes localized in regions of diameter d at times 0, ρ_0, σ_0 with corresponding real intermediate propagating particles.

As in Sec. V.A, we may write

$$W(\rho, \sigma) = \int w(\rho, \sigma, \mathbf{K}_1, \mathbf{K}_2, \mathbf{K}_3)\,d\mathbf{K}_1\,d\mathbf{K}_2\,d\mathbf{K}_3.$$

The function w is appreciable only for

$$|\boldsymbol{\rho} - (\mathbf{K}_1/K_{40})\rho_0| \leqslant d,$$
$$|\boldsymbol{\sigma} - (\mathbf{K}_1/K_{20})\sigma_0| \leqslant d,$$
$$|\boldsymbol{\rho} - \boldsymbol{\sigma} - (\mathbf{K}_3/K_{30})(\rho_0 - \sigma_0)| \leqslant d.$$

At the limit when d is negligible compared to ρ_0, σ_0, these equations are those given in[10] for "point processes," and indeed correspond to classical kinematics.

Other cases. Other cases of Landau-type behavior can be treated along the same lines.

Unstable intermediate particles are related to a behavior of type (76) with a propagator $D_i(k_i)$ corresponding to an unstable particle

$$D_i(k_i) = (k_i^2 - m_i^2 + i\gamma)^{-1}.$$

However, we are restricted to the cases when only one line joins two bubbles in the graph of the singularity.

VI. EVOLUTION OF STATES

A. Preparation of a State

We have written in Eq. (73) the classical current intensity of a particle M produced in a scattering $A + B \to A_1 + M$, for given probability densities or efficiencies of particles A, B, A_1.

Under special conditions ($y_0 \gg d$), an approximation has been obtained in Eq. (74). The particle M can then be considered as freely propagating.

We now assume furthermore that the first final particle A_1 has actually been measured by our apparatus. This new information leads us to consider the new current intensity j_{int} for particle M:

$$j_{\text{int}}(K, y) = \frac{1}{W_1}\,j_{\text{int}}(K, y), \tag{80a}$$

where $j_{\text{int}}(K, y)$ is defined in Eq. (74a) and W_1 in Eq. (74b), the new normalization being as expected:

$$\int j_{\text{int}}'^{0}(K, y)\,dK\,d\mathbf{y}|_{y_0 \gg d} = 1, \tag{80b}$$

where

$$j(K, y) = \exp\,[(-\gamma/K_0)y_0]\,j'(K, y).$$

In dividing by W_1, we have used the new information that particle M has actually been produced.

It can now be easily seen that, under classical-type conditions, S-matrix theory actually leads to a classical-type description of the preparation of a state.

In fact, for $\rho_0 \gg d$, the factor $\theta(y_0 - x_0 + \rho_0)$ in Eq. (75) can be replaced by unity and

$$\exp\,[-\gamma(y_0 - x_0 + \rho_0)/K_0]$$

by $\exp\,(-\gamma\rho_0/K_0)$.

These approximations amount to replacing the factor

$$\frac{1}{k^2 - m^2 + i\gamma}\,\frac{1}{k'^2 - m^2 - i\gamma}$$

in Eq. (58) by

$$\exp\left(-\frac{\gamma\rho_0}{K_0}\right)\delta(k^2 - m^2)\delta(k'^2 - m^2).$$

If here, too, the final particle A_1 has being detected, the global transition probability of the scattering $A + B + C \to A_1 + B_1 + C_1$ can be calculated as the transition probability of the scattering $M + C \to B_1 + C_1$ where the state of particle M is given through the density matrix ζ_M:

$$\zeta_M(\mathbf{k}, \mathbf{k}') = \exp\,(-\gamma\rho_0/K_0)(1/W_1)$$
$$\times \int \zeta_a(\mathbf{p}, \mathbf{p}')\zeta_b(\mathbf{q}, \mathbf{q}')F_a(\mathbf{p}_1, \mathbf{p}_1')t(\mathbf{p}, \mathbf{q}, \mathbf{p}_1, \mathbf{k})$$
$$\times t^*(\mathbf{p}', \mathbf{q}', \mathbf{p}_1', \mathbf{k}')\delta(p + q - p_1 - k)$$
$$\times \delta(p' + q' - p_1' - k')$$
$$\times \frac{d\mathbf{p}}{2p_0}\frac{d\mathbf{p}'}{2p_0'}\frac{d\mathbf{q}}{2q_0}\frac{d\mathbf{q}'}{2q_0'}\frac{d\mathbf{p}_1}{2p_{10}}\frac{d\mathbf{p}_1'}{2p_{10}'}, \tag{81}$$
$$k_0 = (\mathbf{k}^2 + m^2)^{\frac{1}{2}}, \quad k_0' = (\mathbf{k}'^2 + m^2)^{\frac{1}{2}},$$
$$K_0 = \tfrac{1}{2}(k_0 + k_0'),$$

where W_1 is the transition probability of the scattering $A + B \to A_1 + M$, for A, B, A_1 defined by ζ_a, ζ_b, F_a and for M defined through the efficiency matrix:

$$F_{M}(\mathbf{k}, \mathbf{k}') = 2k_0\delta(\mathbf{k} - \mathbf{k}').$$

We may then describe the process by saying that we have prepared particle M in the state defined in Eq. (81).

This can be extended to processes of multiple successive scatterings.

B. The Straight Track

As an example, we answer the following simple problem: does S-matrix theory describe the creation of a straight track in a bubble chamber?

In the framework of quantum mechanics, where one uses some equations for the evolution of states in time, this problem has been solved.[15,16]

We will give here the classical description of the process, and because of the results of Sec. VI.A, it will easily be seen that S-matrix theory actually leads to that description.

We consider an α particle which has been emitted in the chamber by a nucleus. Its probability density is constant inside the bubble chamber, zero outside, after its emission. The momentum distribution is isotropic and is usually peaked around some value of $|\mathbf{P}|$. It also decreases exponentially with time.

The chamber is filled with atoms which are described by similar probability densities.

After a while, we see an ionized atom and an electron. If we call $j_a(P, x)$, $j_b(Q, x)$ the current intensities of the α particle and the atom, respectively, $E_a(P_1, x)$, $E_b(Q_1, x)$ the efficiencies for the detection of the ionized atom and electron, respectively, we get, according to formula (73), the α-particle current intensity after collision:

$$\begin{aligned} j^1_{\text{int}}(K, y) &= \frac{1}{W_1}\int j_a(P, x) j_b(Q, x) E_a(P_1, x) E_b(Q_1, x) \\ &\times \delta\left(\mathbf{x} - \mathbf{y} - \frac{\mathbf{K}}{K_0}(x_0 - y_0)\right) \exp\left(-\frac{\gamma(y_0 - x_0)}{K_0}\right) \\ &\times \theta(y_0 - x_0)\delta(k^2 - m^2) w(\mathbf{P}, \mathbf{Q}, \mathbf{P}_1, \mathbf{Q}_1, \mathbf{K}) \\ &\times \delta(P + Q - P_1 - Q_1 - K)\, dP\, dQ\, dP_1\, dQ_1\, dx \\ &\times \frac{1}{2K_0}\delta(K^2 - m^2)\theta(K_0). \end{aligned} \tag{82}$$

The process of seeing, in S-matrix theory, is akin to the process of trackmaking and should be, of course, treated along the same lines. A complete measurement theory should involve these ideas in a "bootstrap" sort of way.

If E_a, E_b are rapidly decreasing in $\mathbf{x} - (\mathbf{P}_1/P_{10})x_0$, $\mathbf{x} - (\mathbf{Q}_1/Q_{10})x_0$ and have no overlap in velocities $\mathbf{P}_1/P_{10}$, $\mathbf{Q}_1/Q_{10}$, the region of the first interaction is well defined and the product E_aE_b rapidly decreasing in x in all directions.

Now we see a second group of ionized atoms and electrons. Then the current of the α particle, after the second collision, will be

$$\begin{aligned} j^{(2)}_{\text{int}}(L, z) &= (1/W_1W_2)\int j^1_{\text{int}}(K, y) j_b(R, y) E_a(R_1, y) E_b(S_1, y) \\ &\times \delta(\mathbf{y} - \mathbf{z} - (\mathbf{L}/L_0)(y_0 - z_0))\theta(z_0 - y_0) \\ &\times \exp\left[-\gamma(z_0 - y_0)/L_0\right]\delta(L^2 - m^2) \\ &w(\mathbf{K}, \mathbf{R}, \mathbf{R}_1, \mathbf{S}, \mathbf{L})\delta(K + R - R_1 - S_1 - L) \\ &\times dK\, dR\, dR_1\, dS_1\, dy\theta(L_0)(1/2L_0). \end{aligned} \tag{83}$$

Here, again, the product $E_a(R_1, y)E_b(S_1, y)$ defines the region of the second interaction.

We substitute the expression of $j(K, y)$ given by (82) into Eq. (83). Because of the factor $\delta(\mathbf{x} - \mathbf{y} - (\mathbf{K}/K_0)(x_0 - y_0))$,

$$\frac{\mathbf{K}}{K_0} = \frac{\mathbf{y} - \mathbf{x}}{y_0 - x_0}$$

is well enough defined. Then, because of the shape of $w(\mathbf{K}, \mathbf{R}, \mathbf{R}_1, \mathbf{S}_1, \mathbf{L})$, the current density $j^{(2)}_{\text{int}}(L, z)$ will be peaked in the region defined by

$$\frac{\mathbf{L}}{L_0} \sim \frac{\mathbf{K}}{K_0} \sim \frac{\mathbf{y} - \mathbf{x}}{y_0 - x_0}.$$

(This is the well-known fact that, if the particle α has a well-enough defined velocity, this velocity cannot be appreciably changed.)

Now since $j(L, z)$ is peaked around some value of $\mathbf{L}/L_0$, the probability of a new interaction will be peaked for this new interaction happening around the direction given by the line joining the localized regions of the two first scatterings, and so on, which explains the occurrence of a straight track.

Owing to the results of Sec. V.A, the same result will hold in S-matrix theory: the probability of seeing a new interaction is peaked in the direction of the first two.

VII. CONCLUSION

The following general hypotheses have been made. The S matrix is assumed to conserve energy–momentum, which yields energy–momentum conservation and translational invariance of the transition probabilities.

[15] N. F. Mott, Proc. Roy. Soc. (London) **126**, 79 (1929).

[16] For the general study of many problems similar to those studied in our work in the framework of quantum mechanics, we refer to A. Messiah, *Mécanique quantique* (Dunod Cie., Paris, 1965).

TABLE I. Results for the S matrix.

	Approximations	Consequences
Invariant density or efficiency functions	$\frac{1}{m} \ll A_x$	$j_I(P,x) \approx j_F(P,x)$
$j_I(P,x), j_F(P,x) = g_F\left(\mathbf{P}, \mathbf{x} - \frac{\mathbf{P}}{P_0} x_0\right)$	$\frac{1}{m} \ll A_x$	$0 \leqslant g_F(\mathbf{P}, \mathbf{y}) \leqslant 1$
$\times\ \delta(P^2 - m^2)\theta(P_0)$	$\frac{1}{A_p} \ll A_x$	
Single scattering	$\left\lvert\frac{\nabla t}{t}\right\rvert \ll A_x$ 1st order	coarse-grained locality
	0th order	locality
Double scattering	$\frac{K_0}{\gamma} \ll A_x \leqslant A_p$	bump in the cross sections
	$\frac{1}{A_p} \ll \frac{K_0}{\gamma} \ll A_x$	on-mass-shell kinematical condition
	$\frac{1}{m} \ll A_x \leq d \ll \rho_0 \leqslant \frac{K_0}{\gamma}$	propagation of a real intermediate particle

A property of the decomposition in connected elements is also assumed to hold and yields a cluster property of the transition probabilities.

The other results can be summarized in Table I.

In this table, A_x and A_p are the space and momentum deviations of the density and efficiency functions, respectively. Under the approximations made, they enjoy the properties of classical probability densities and measurement efficiencies, respectively.

The table then shows under which conditions coarse-grained locality or locality of an interaction is obtained.

A polelike behavior of the connected elements is assumed in a weak form (analyticity hypotheses are not necessary) and, under the conditions of the table, leads to the usual classical cases mentioned. The 4-vector K is the momentum of the "intermediate" particle. The first case is the observation of a bump of width γ/K_0 in the cross sections, for instance the case of the N^*. In the second case, an on-mass-shell kinematical condition is written, as in the case of the Σ^0. The last case mentioned corresponds to two successive scattering processes which are localized in space–time regions of diameter d, separated by a 4-vector ρ, with the propagation of a real intermediate particle, for instance, a neutron.

Landau-type behavior of the connected elements can also lead to classical-type formulas of multiple successive scatterings.

All the above results allow one to understand how S-matrix theory actually leads to the usual classical description of the preparation of a state, and generally to the usual classical description of processes, involving the usual classical concepts and formulas.

These results are satisfactory and justify *a posteriori* general hypotheses on S-matrix theory and on the correspondence between the S matrix and classical description of states.

Dynamical aspects of interaction processes are not studied. It is the aim of theories involving stronger hypotheses to obtain the corresponding results. For instance, axiomatic field theory[17] or analytic S-matrix theory are two theories which contain, in particular, all the features of S-matrix theory used here and are, of course, much more restrictive.

Thus we think it is useful to know what part of the hypotheses of such theories corresponds to the kinematical aspects of the description of processes, and to understand precisely how and when they lead to the classical description, which is the only ground on which theory and experiment meet.

Note Added in Proof: Various new results on asymptotic space–time properties in S-matrix theory have been obtained recently by C. Chandler and H. P. Stapp [J. Math. Phys. **10**, 826 (1969)] and D. Iagolnitzer and H. P. Stapp (report of work prior to publication). A general review of space–time properties in S-matrix theory and the current status of the results reported in this paper were presented by the author at the 1968 Boulder Institute for Theoretical Physics.

ACKNOWLEDGMENTS

I would like to thank M. Froissart who directed this work for providing the main ideas and for his generous and continuous help.

[17] K. Hepp, J. Math. Phys. **6**, 1762 (1965), and references quoted therein.

I would like to thank R. Balian, J. Bros, A. Messiah, D. Ruelle, R. Stora, and D. Williams for interesting discussions which are at the origin of some parts of this work.

APPENDIX A: SINGULARITIES

This is a short critical review of what has been or can be said about the relation between timelike cluster properties of the transition amplitudes and one-particle singularities or more generally Landau-type singularities of the connected matrix elements.

It is thus distinct from the general purpose of this work which is to obtain the classical formulas.

Derivation of the Propagator

We consider, for the sake of simplicity, a scattering $A + B + C \to A_1 + B_1 + C_1$, where the particle states are defined through the wavefunctions $\varphi_a(\mathbf{p})$, $\varphi_b(\mathbf{q})$, $\varphi_c(\mathbf{r})$, $\psi_a(\mathbf{p}_1)$, $\psi_b(\mathbf{q}_1)$, $\psi_c(\mathbf{r}_1)$.

The kinematical and other conditions allow the possibility of scatterings $A + B \to A_1 + M$, $C + M \to B_1 + C_1$ for some particle M. No other possibility exists.

We denote by A^ρ the state of particle A translated through the 4-vector ρ and we define the following quantities:

$$L(\rho) = \langle ABC^\rho | \, T \, | A_1 B_1^\rho C_1^\rho \rangle,$$
$$N(\rho) = \langle C^\rho M | \, T \, | B_1^\rho C_1^\rho \rangle,$$

where the state of particle M is defined through its wavefunction

$$\varphi_M(\mathbf{k}) = \langle AB | \, T \, | A_1 \mathbf{k} \rangle,$$
$$\int |\varphi_M(\mathbf{k})|^2 \frac{d\mathbf{k}}{2k_0} = W_1,$$

where W_1 is the transition probability from A, B to A_1 and M, the states of particles A, B, A_1 being defined above, and all final states of M being considered.

We then define

$$H(\rho) = L(\rho) - \theta(\rho_0) N(\rho).$$

For large $|\rho_0|$, the property (P) stated in Sec. II.D means that $|L(\rho)|$ should behave like $|N(\rho)|$ for $\rho_0 > 0$, and be negligible for $\rho_0 < 0$. Assuming furthermore that it also holds for the transition amplitudes, it means that $H(\rho)$ should be negligible for large $|\rho_0|$. We do not know if and how it is possible to derive it. As it is stated here, it is a strong hypothesis.

Different kinds of conditions can be stated. For instance, Wanders[4] requires the rather weak, but yet arbitrary, condition:

$$\int |H(\rho)|^2 \, d\rho < +\infty,$$

as opposed to

$$\int |N(\rho)|^2 \, d\rho = +\infty, \quad \int |N(\rho)|^2 \, d\boldsymbol{\rho} = \text{const.}$$

From that condition, the polelike behavior of the connected matrix elements is derived:

$$T(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) = t(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) \times \delta(p + q + r - p_1 - q_1 - r_1),$$
$$t(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) = \frac{(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1)}{k_0 - (k^2 + m^2 + i\epsilon)^{\frac{1}{2}}},$$

where

$$k = p + q - p_1$$

and $\mathcal{R}$ has a suitable regularity property.

This polelike behavior can also be derived[7,8] from analyticity (and unitarity[6]), the function $\mathcal{R}$ being then analytic.

Some authors[5] like better to consider, instead of the quantities $L(\rho)$, $N(\rho)$, $H(\rho)$, the quantities $N(0)$ and

$$L'(\rho_0) = \int T(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) \times \varphi_a^*(\mathbf{p}) \varphi_b^*(\mathbf{q}) \varphi_c^*(\mathbf{r}) \psi_a(\mathbf{p}_1) \psi_b(\mathbf{q}_1) \psi_c(\mathbf{r}_1) \times \exp\{i\rho_0[k_0 - (\mathbf{k}^2 + m^2)^{\frac{1}{2}}]\} \pi \frac{d\mathbf{p}}{2p_0} \pi \frac{d\mathbf{q}}{2q_0}.$$

Their requirement, claimed to be "physically reasonable," is that—at least for test functions of $\mathcal{S}$ such that furthermore all velocities cannot be equal all together—the quantity

$$H'(\rho_0) = L'(\rho_0) - \theta(\rho_0) N(0)$$

should go rapidly to zero for large $|\rho_0|$. To us, the restriction of the test functions given here may be reasonable enough, but not the substitution of the quantity H' for H.

The polelike singularity is derived here too, the Fourier transform $\tilde{L}'(\xi)$ of $L'(\rho_0)$ being the product of the propagator $1/(\xi + i\epsilon)$ with a C^∞ function.

Converse Part

Conversely, let us consider the hypotheses of a polelike behavior of the t-matrix elements in the following form:

$$t(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) = \frac{\mathcal{R}(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1)}{k_0 - (k^2 + m^2)^{\frac{1}{2}} + i\epsilon},$$

where $\mathcal{R}$ is some function, satisfying, furthermore, the condition

$$\mathcal{R}(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1)_{k_0 = (k^2 + m^2)^{\frac{1}{2}}} = (1/2k_0) t(\mathbf{p}, \mathbf{q}, \mathbf{p}_1, \mathbf{k}) t(\mathbf{k}, \mathbf{r}, \mathbf{q}_1, \mathbf{r}_1).$$

One gets

$$L(\rho) = \int \mathcal{S}(\mathbf{k}, \mathbf{k}_0) \frac{1}{k_0 - (k^2 + m^2)^{\frac{1}{2}} + i\epsilon} \times \exp(i\rho k)\, d^4k,$$

$$\mathcal{S}(k) = \int \mathcal{R}(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) \varphi_a^*(\mathbf{p}) \varphi_b^*(\mathbf{q}) \varphi_c^*(\mathbf{r}) \times \psi_a(\mathbf{p}_1) \psi_b(\mathbf{q}_1) \psi_c(\mathbf{r}_1) \delta(p + q - p_1 - k) \times \delta(k + r - q_1 - r_1) \pi \frac{d\mathbf{p}}{2p_0} \pi \frac{\mathbf{p}_1}{2p_{10}},$$

$$N(\rho) = \int \mathcal{S}(\mathbf{k}, k_0) \delta(k_0 - (k^2 + m^2)^{\frac{1}{2}}) \exp(i\rho k)\, dk,$$

$$\theta(\rho_0) N(\rho) = \int \mathcal{S}(\mathbf{k}, (k^2 + m^2)^{\frac{1}{2}}) \frac{1}{k_0 - (k^2 + m^2)^{\frac{1}{2}} + i\epsilon} \times \exp(i\rho k)\, dk,$$

$$L'(\rho_0) = \int \mathcal{S}(\mathbf{k}, k_0) \frac{1}{k_0 - (k^2 + m^2)^{\frac{1}{2}} + i\epsilon} \times \exp\{i\rho_0 [k_0 - (k^2 + m^2)^{\frac{1}{2}}]\}\, dk.$$

By making different kinds of hypotheses both on the nature of the function $\mathcal{R}$ and on the test functions, it is possible to get results.

For instance, $H'(\rho_0)$ can be written as

$$H'(\rho_0) = \int (\sum(\xi) - \sum(0)) \frac{1}{\xi + i\epsilon} \exp(i\rho_0 \xi)\, d\xi,$$

where

$$\sum(\xi) = \int \mathcal{S}(\mathbf{k}, k_0) \delta(k_0 - (k^2 + m^2)^{\frac{1}{2}} - \xi)\, d^4k.$$

By assuming that $\mathcal{R}$ is a C^∞ function and considering test functions in $\mathcal{S}$, the rapid decrease of $H'(\rho_0)$ for large $|\rho_0|$ can be deduced.

Although the consideration of $H(\rho_0)$ is not so easy, conclusions can also be drawn from the expression

$$H(\rho_0) = \int \frac{\mathcal{S}(\mathbf{k}, k_0) - \mathcal{S}(\mathbf{k}, (k^2 + m^2)^{\frac{1}{2}})}{k_0 - (k^2 + m^2)^{\frac{1}{2}} + i\epsilon} \exp(i\rho k)\, dk.$$

Unstable "Intermediate" Particle

The case when the t-matrix elements behave like

$$t(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) = \frac{\mathcal{M}(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1)}{k^2 - m^2 + i\gamma},$$

with some hypothesis on the behavior of $\mathcal{M}$, can also be studied[7,8] (e.g., if $\mathcal{M}$ is analytic and factorizable in two parts for $k^2 = m^2 + i\gamma$) by comparison of $L(\rho)$ [respectively, $L'(\rho_0)$] for large $|\rho_0|$, $|\gamma\rho_0/k_0| \sim 1$ with $N_\gamma(\rho)\theta(\rho_0)$ [respectively, $\theta(\rho_0)N_\gamma(0)$], where

$$\theta(\rho_0) N_\gamma(\rho) = \int \varphi(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{p}_1, \mathbf{q}_1, \mathbf{r}_1) t(\mathbf{p}, \mathbf{q}, \mathbf{p}_1, \mathbf{k}) t(\mathbf{k}, \mathbf{r}, \mathbf{q}_1, \mathbf{r}_1) \times \delta(p + q - p_1 - k) \theta(\rho_0) \times \delta(k + r - q_1 - r_1) \pi \frac{d\mathbf{p}}{2p_0} \pi \frac{d\mathbf{p}_1}{2p_{10}} \times \exp(-\gamma\rho_0/k_0) \frac{d\mathbf{k}}{2k_0}.$$

This case may be treated along the same lines as the "stable" case.

Landau-type Case

The case of a Landau-type behavior can also be treated in a similar way. A simple qualitative hint[10] indicates why Landau singularities in the physical region can be related to physical possible processes.

In general, a predominance rule of all physically possible processes with all possible intermediate particles should be stated.

Some progress seems to be made from different kinds of hypotheses.

Analyticity hypotheses with simple conjectures lead to interesting results.[18]

Hypotheses of rapid decrease in time of the part of the amplitude remaining after all terms corresponding to physically possible processes have been subtracted out may seem "physically reasonable" and promising.

APPENDIX B: ABOUT WIGNER FUNCTIONS

Definition

There has been a lot of literature about the Wigner or other "quasiprobability" functions. Curiously enough, people usually limit themselves to the case of a density matrix—and do not study the more general case of an efficiency matrix!

Authors then consider the following correspondence:

$$\zeta \to \mathcal{S}(\lambda, \mu) = \mathrm{Tr}\, \zeta \exp[i(\lambda \mathbf{P}_{0p} + \mu \mathbf{X}_{0p})^{\sim}],$$

where $^{\sim}$ is the closure of the operator. Then the Wigner function is the Fourier transform of $\mathcal{S}(\lambda, \mu)$:

$$g_W(P, x) = \int \mathcal{S}(\lambda, \mu) \exp[-i(\lambda P + \mu x)]\, d\lambda\, d\mu.$$

The above correspondence is more generally an a^*-isomorphism of the algebra of Hilbert–Schmidt operators on the Hilbert space of square-integrable

[18] F. Pham, "Singularités des processus de diffusion multiple," CERN Preprint 65/487/5-TH651, 1965.

functions into the algebra of square-integrable complex-valued phase-space functions [with multiplication defined in Eq. (32)].[19]

Discussion of Equation (29)

To some extent, Eq. (29) is related to von Neumann's[20] construction of sets of two commuting operators which approximate X_{0p} and P_{0p} and which, instead of having a continuous spectrum as the usual position and momentum operators, have discrete eigenvalues, the product of intervals between two eigenvalues of each being larger or equal to one.

To prove Eq. (29) as recalled in Sec. III.B.2, one may write the inequality

$$0 \leq \langle \chi_0 | F | \chi_0 \rangle \leq \langle \chi_0 | \chi_0 \rangle$$

for a minimal wavepacket χ_0:

$$\chi_0(\mathbf{p}) = (2p_0)^{\frac{1}{2}} \left(\frac{B_x}{\sqrt{2\pi}} \right)^{\frac{3}{2}} \exp(i\mathbf{p}\mathbf{x}_0) \times \exp[-\tfrac{1}{2}B_x^2(\mathbf{p} - \mathbf{P}_0)^2].$$

Equation (29) follows for $B_p = (2B_x)^{-1}$, $B_pB_x = \frac{1}{2}$. The generalization to $B_pB_x \geq \frac{1}{2}$ is then trivial [a convolution with $B_pB_x \geq \frac{1}{2}$ can be separated into the product of convolutions with $B_p'B_x' = \frac{1}{2}$ and another one with positive (exponential) functions].

We may also obtain this directly by using the inequality

$$0 \leq \operatorname{Tr} F\zeta_0 \leq 1,$$

valid for all density matrix ζ_0, then choosing

$$\zeta_0(\mathbf{p}, \mathbf{p}') \propto \exp[i(\mathbf{p} - \mathbf{p}')\mathbf{x}_0] \exp[-\tfrac{1}{4}B_x^2(\mathbf{p} - \mathbf{p}')^2] \times \exp\{-[\tfrac{1}{2}(\mathbf{p} + \mathbf{p}') - \mathbf{P}_0]^2 B_p^{-2}\}(2p_0)^{\frac{1}{2}}(2p_0')^{\frac{1}{2}},$$

which is a kernel of density matrix if and only if $B_xB_p \geq \frac{1}{2}$.

Some authors define new kinds of "quasiprobability" functions instead of the Wigner function.

For instance, what Bopp has written[21] is, as a matter of fact, nothing else than the convolution of g_W through $\tau_l(\mathbf{x})\tau_{1/l}(\mathbf{P})$ where l is some "fundamental" length. However, the physical meaning as well as the exact equation (29) is not clearly given. Furthermore, we do not follow him on the ground of "fundamental" length l. Equation (29) is valid for all $\{B_x, B_p: B_xB_p \geq \frac{1}{2}\}$.

Other authors[22] prefer to say that instead of the above correspondence,

$$\zeta \to S(\lambda, \mu) = \operatorname{Tr} \zeta \exp[i(\lambda\mathbf{P}_{0p} + \mu\mathbf{X}_{0p})^{\sim}],$$

they will consider correspondences using other "orderings" of $\mathbf{P}_{0p}$ and $\mathbf{X}_{0p}$ or combinations, i.e., things like $\exp(i\lambda\mathbf{P}_{0p}) \exp(i\mu\mathbf{X}_{0p})$, etc.

If one defines dimensionless operators p_{0p} and x_{0p} using $p_{0p} = lP_{0p}$, $x_{0p} = 1/lX_{0p}$ (l is some length), and

$$\hat{A} = (\mathbf{x}_{0p} + i\mathbf{p}_{0p})/\sqrt{2},$$
$$\hat{A}^+ = (\mathbf{x}_{0p} - i\mathbf{p}_{0p})/\sqrt{2},$$
$$\alpha = -\lambda/(l\sqrt{2}) + i\mu(l/\sqrt{2}),$$

one gets

$$-\alpha^*\hat{A} + \alpha\hat{A}^+ = \lambda P_{0p} + \mu X_{0p},$$

$$\exp(-\alpha^*\hat{A}) \exp(\alpha\hat{A}^+) = \exp(-\alpha^*\hat{A} + \alpha\hat{A}^+) \exp(-|\alpha|^2) = \exp[i(\lambda\mathbf{P}_{0p} + \mu\mathbf{X}_{0p})] \exp[-(\lambda^2/2l^2 + \mu^2\tfrac{1}{2}l^2)].$$

Thus the new "quasiprobability" function defined by Glauber *et al.* through

$$\zeta \to S(\lambda, \mu) = \operatorname{Tr} \zeta \exp(-\alpha^*\hat{A}) \exp(\alpha\hat{A}^+)$$

is also just the convolution of the Wigner function with $\tau_l(\mathbf{x})\tau_{1/l}(\mathbf{P})$ as in Bopp's case. Same comment as about Bopp's case applies.

Positive Wigner Functions

Let us end now through a short discussion of Eqs. (26), (27), and (28) where cases when Wigner functions are positive were studied.

The function g_0 defined in Eq. (26) can be proved to be the Wigner function of the density matrix ζ_0 defined in Eq. (27) by using, for instance, a theorem by Bloch concerning the probability law of a combination of momentum and position.[23]

In the special case studied here, the Wigner function is formally identical with the probability density of the classical case. It can be easily understood by considering that one has to minimize in the classical case $\int g \ln g$ and in the quantum case $\operatorname{Tr} \zeta \ln \zeta$.

Then

$$\operatorname{Tr} \zeta \ln \zeta = \int (\zeta)_W(P, x)(\ln \zeta)_W(P, x)\, dP\, dx,$$
$$(P_{0p})_W = P,$$
$$(X_{0p})_W = x.$$

In this special case, $(\ln \zeta)_W(P, x) \propto \ln (\zeta)_W(P, x)$. The equations of the classical and quantum mechanical case then become identical.

[19] J. C. T. Pool, J. Math. Phys. 7, 66 (1966).

[20] J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Princeton, N.J., 1955), p. 398–416.

[21] F. Bopp, Ann. Inst. Poincaré **15**, 81 (1956).

[22] See, for instance, C. L. Mehta, "Coherence and Statistics of Radiation," in *Lectures in Theoretical Physics, Vol. VIIC*, W. E. Britten, Ed. (University of Colorado Press, Boulder, Colo., 1965).

[23] See A. Messiah, *Mécanique quantique* (Dunod Cie., Paris, 1965), Vol. I, p. 382.

Partial-Wave Expansion in the Crossed Channel for Scattering Amplitudes Invariant under the Galilei Group*

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(Received 5 September 1968)

A partial-wave analysis in the crossed channel is performed for a Galilean-invariant scattering matrix using the irreducible unitary representations of the Euclidean group in two dimensions. As in the relativistic case, a formula is obtained which is useful in determining the high-energy behavior of the scattering amplitude for fixed-momentum transfer. In particular, the Born term is shown to correspond to a δ function in this representation. Moreover, this parametrization is related by a group contraction to the corresponding background term of the relativistic case.

1. INTRODUCTION

In the Regge approach to relativistic two-body scattering, an expansion is obtained for the amplitude $T(s, t)$ by a Sommerfeld–Watson transformation. One gets, typically, for unit masses

$$T(s,t) = \sum_i \beta_i(t) P_{\alpha_i(t)}\left(-1 - \frac{2s}{t-4}\right) + \frac{1}{i}\int_{-\infty}^{+\infty} d\sigma \frac{G(t,\sigma)}{\cosh(\pi\sigma)} P_{-\frac{1}{2}+i\sigma}\left(-1 - \frac{2s}{t-4}\right), \tag{1.1}$$

where s and t are the usual Mandelstam variables. A group-theoretic interpretation can be given to this formula which is identified with a partial-wave analysis performed in the t channel while remaining in the physical region of the s channel[1,2] and it provides a very interesting link between Regge poles and certain representations of the Poincaré group. There seems to be a general feeling that such a link does not exist in the case of nonrelativistic scattering, where the group of invariance is the Galilei group.[3] We believe that this is due to the fact that people have been seeking expressions looking exactly the same as (1.1). In this connection it is useful to recall that (1.1) contains the Regge poles of the crossed channel and not the poles originally obtained by Regge.[4] Moreover, in nonrelativistic scattering there is a fundamental difference between the s and t channels, the latter being a purely kinematical concept.

For these two reasons one should not expect to reach a result exactly similar in structure to (1.1) in the Schrödinger theory. We will show that a partial-wave analysis in the t channel using the Galilei group leads to an expression whose main difference from (1.1) is the replacement of Legendre polynomials by Bessel functions. This is quite natural, since in the contraction of the Poincaré group to the Galilei group the Legendre functions go to the Bessel functions. Furthermore, the Born term, which determines the high-energy behavior at fixed-momentum transfer corresponds to a pole in the continuous parameter in which the expansion is made.

2. GROUP-THEORETICAL COUPLING OF INITIAL AND FINAL STATES

We recall that the Galilei group G is the set of elements of the form

$$g = (a^0, \mathbf{a}, \mathbf{v}, R). \tag{2.1}$$

This group acts on the coordinates $(t, \mathbf{x})$ of space–time according to

$$\begin{aligned} \mathbf{x}' &= R\mathbf{x} + \mathbf{v}t + \mathbf{a}, \\ t' &= t + a^0, \end{aligned} \tag{2.2}$$

where a^0 and $\mathbf{a}$ are time and space translations, respectively, $\mathbf{v}$ a velocity, and R a rotation.

Bargmann[5] has demonstrated that all irreducible unitary continuous projective representations of the covering group of the Galilei group $\tilde{G}$ are characterized by the system of factors

$$\omega(g', g) = \exp\left[\tfrac{1}{2}im(\mathbf{a}' \cdot R'\mathbf{v} - \mathbf{v}' \cdot R\mathbf{a} + a^0\mathbf{v}' \cdot R'\mathbf{v})\right]. \tag{2.3}$$

The universal covering group $\tilde{G}$ is obtained by performing the usual substitution $R \to A \in SU_2$. As shown by Bargmann, the parameter m, if greater

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[1] H. Joos, in *Boulder Lectures in Theoretical Physics, Vol. VII* (University of Colorado Press, Boulder, Colo., 1964), p. 132.
[2] M. Toller, Nuovo Cimento **37**, 631 (1965).
[3] J.-M. Levy-Leblond, Nuovo Cimento **45A**, 772 (1966); L. H. Ryder, *ibid.* **52A**, 879 (1967).
[4] T. Regge, Nuovo Cimento **14**, 951 (1959); Nuovo Cimento **18**, 947 (1960).
[5] V. Bargmann, Ann. Math. **59**, 1 (1954).

than zero, can be interpreted as the mass of the particle.

We give a brief sketch on how to get the irreducible unitary representations of $\tilde{G}$ following the method of Mackey.[6] (For details see Refs. 6–8.)

The characters of the space–time translations $(a^0, \mathbf{a}, \mathbf{0}, 1)$ are the usual ones,

$$e^{i(p^0a^0-\mathbf{p}\cdot\mathbf{a})},$$

and the energy–momentum $p = (p^0, \mathbf{p})$ transforms according to

$$\begin{aligned} p^{0\prime} &= p^0 + \mathbf{v}\cdot R\mathbf{p} + \tfrac{1}{2}m\mathbf{v}^2, \\ \mathbf{p}' &= R\mathbf{p} + m\mathbf{v}. \end{aligned} \tag{2.4}$$

(We always adopt, where possible, the four-dimensional notation.)

It can be easily checked that

$$2mp^0 - \mathbf{p}^2 = B \tag{2.5}$$

is invariant under the transformation (2.4) and, conversely, two four-vectors, lying in the same orbit corresponding to a fixed value of B, can be connected by a transformation (2.4). Thus the number B is one of the labels of the irreducible unitary representations. We can then parametrize each orbit by choosing a fixed vector h and a transformation M_p of the type (2.4) such that $p = M_p h$. [We will always denote by M the elements of the form $(0, \mathbf{0}, \mathbf{v}, A)$, written simply as $(\mathbf{v}, A)$.]

The irreducible unitary representations can now be written in the space of the square-integrable functions on the orbit with respect to the measure $d_4p\delta(2mp^0 - \mathbf{p}^2 - B)$:

$$(U(a, \mathbf{v}, A)f)(M_p) = e^{ip\cdot a}Q(M_p^{-1}MM_{M_p^{-1}})f(M_{M_p^{-1}}), \tag{2.6}$$

where we have put $M = (\mathbf{v}, A)$. The set of Q's form an irreducible unitary representation of the little group G_h of h, to which $M_p^{-1}MM_{M_p^{-1}}$ belongs. More generally, Mackey[6] works with the functions defined on the group $\tilde{G}$ and the representation is the left-regular representation. The link between the functions on the group and $f(M_p)$ is given by the so-called "Q covariance along left cosets"[9] expressed by

$$f(M\varphi) = Q^{-1}(\varphi)f(M)$$

if $\varphi \in G_h$.

We now have to distinguish two different cases: if m is not zero, looking at (2.4), one sees that G_h is isomorphic to SU_2. Accordingly, the Q's are the standard D^s matrices and s is interpreted as the spin of the particle. In the following, a convenient parametrization of the orbit will be the choice

$$h = \left(\frac{B}{2m}, \mathbf{0}\right) \quad \text{and} \quad M_p = \left(\frac{\mathbf{p}}{m}, 1\right). \tag{2.7}$$

Then one obtains

$$M_p^{-1}MM_{M_p^{-1}} = (\mathbf{0}, A).$$

If $m = 0$, G_h is the set of $(0, \mathbf{0}, \mathbf{v}, A)$ such that

$$\mathbf{h}\cdot\mathbf{v} = 0 \quad \text{and} \quad R(A)\mathbf{h} = \mathbf{h}.$$

This group is isomorphic to the two-sheeted covering group of the Euclidean group in two dimensions E_2. The irreducible unitary representations of E_2 are recalled in the Appendix. If the representation of the little group is one-dimensional (the so-called finite-spin case), one has simply

$$Q^{(n)}(M_p^{-1}MM_{M_p^{-1}}) = e^{in\theta(M_p^{-1}MM_{M_p^{-1}})}.$$

In the case of infinite-dimensional representations (infinite spin), the representations of $\tilde{G}$ take the form

$$\begin{aligned} &(U(a, \mathbf{v}, A)f)(M_p, C_\mathbf{x}) \\ &\quad = e^{ip\cdot a}e^{iu\cdot\mathbf{x}}D^\epsilon(C_\mathbf{x}^{-1}CC_{C_\mathbf{x}^{-1}})f(M_{M_p^{-1}}, C_{C_\mathbf{x}^{-1}}), \end{aligned} \tag{2.8}$$

where we have let $M_p^{-1}MM_{M_p^{-1}} = (\mathbf{u}, C)$. As it can be seen by direct inspection of (2.4), given any $h = (h^0, \mathbf{h})$ on the orbit with $-\mathbf{h}^2 = B$, a convenient choice of M_p is $(\mathbf{w}, A_p)$, where $R(A_p)\mathbf{h} = \mathbf{p}$ and

$$\mathbf{w} = \mathbf{p}[p^0 - h^0]/\mathbf{p}^2.$$

With this choice, one has

$$\mathbf{u} = R(A_p)^{-1}\left[\mathbf{v} - \frac{\mathbf{v}\cdot\mathbf{p}}{\mathbf{p}^2}\,\mathbf{p}\right]$$

and $C = A_p^{-1}AA_{M_p^{-1}}$. As expected, $\mathbf{u}$ is orthogonal to $\mathbf{h}$, since

$$\mathbf{v} - \frac{\mathbf{v}\cdot\mathbf{p}}{\mathbf{p}^2}\,\mathbf{p}$$

is the component of $\mathbf{v}$ orthogonal to $\mathbf{p}$.

Since we are interested in making a partial-wave analysis in the crossed channel, that is in coupling an incoming particle of mass m with the same outgoing particle, we now focus our attention on performing the reduction of the product of a representation of mass $m \neq 0$ and a representation of mass $-m$ (see Secs. 4 and 7). In this case the product of the factors (2.3) gives unity and one expects to find in the decomposition true representations, i.e., mass-zero

[6] G. Mackey, *The Theory of Group Representations* (The University of Chicago Press, Chicago, 1955).
[7] J.-M. Levy-Leblond, J. Math. Phys. **4**, 776 (1963).
[8] J. Voisin, J. Math. Phys. **6**, 1519 (1965).
[9] P. Moussa and R. Stora, in *Boulder Lectures in Theoretical Physics, Vol. VII* (University of Colorado Press, Boulder, Colo., 1964), p. 37.

representations. In performing the reduction we follow the method of Moussa and Stora,[9] stressing only those points which are particular to our problem.

The product representation is given by

$$(U(a, M)f)_{\sigma_1\sigma_2}(M_{p_1}, M_{p_2}) = e^{i(p_1+p_2)\cdot a} D^{s_1}_{\sigma_1\tau_1}(M_{p_1}^{-1} M M_{M_{p_1}^{-1}}) \times D^{s_2}_{\sigma_2\tau_2}(M_{p_2}^{-1} M M_{M_{p_2}^{-1}}) f_{\tau_1\tau_2}(M_{M_{p_1}^{-1}}, M_{M_{p_2}^{-1}}). \tag{2.9}$$

The orbits are, respectively,

$$2mp_1^0 - |\mathbf{p}_1|^2 = B_1,$$
$$-2mp_2^0 - |\mathbf{p}_2|^2 = B_2,$$

and we denote by h_1 and h_2 the fixed vectors chosen as explained in (2.7). As shown in Ref. 9 the set (M_{p_1}, M_{p_2}) has to be decomposed into double cosets which are characterized by the condition: (M_{p_1}, M_{p_2}) is equivalent to $(M_{p_1'}, M_{p_2'})$ if and only if there exists an M such that $p_1' = M_{p_1}$ and $p_2' = M_{p_2}$. In each double coset one can choose a representative $(M_{\omega_1}, M_{\omega_2})$ with

$$M_{\omega_1} = (\mathbf{v}, 1) \quad \text{and} \quad M_{\omega_2} = (-\mathbf{v}, 1). \tag{2.10}$$

Then, ω_1 and ω_2 are given by

$$\begin{aligned} \boldsymbol{\omega}_1 &= m\mathbf{v}, \\ \omega_1^0 &= (B_1/2m) + \tfrac{1}{2}m\mathbf{v}^2, \\ \boldsymbol{\omega}_2 &= m\mathbf{v}, \\ \omega_2^0 &= -(B_2/2m) - \tfrac{1}{2}m\mathbf{v}^2. \end{aligned} \tag{2.11}$$

If we define

$$\begin{aligned} \pi &= \omega_1 + \omega_2 = \left(\frac{B_1 - B_2}{2m}, 2m\mathbf{v}\right), \\ \chi &= \omega_1 - \omega_2 = \left(\frac{B_1 + B_2}{2m} + m\mathbf{v}^2, \mathbf{0}\right), \end{aligned} \tag{2.12}$$

Eq. (2.4) shows that π transforms with the mass 0 and χ with the mass $2m$. The invariant B of π can be used to label the double cosets. For any (M_{p_1}, M_{p_2}) in the same double coset of $(M_{\omega_1}, M_{\omega_2})$, we introduce

$$\begin{aligned} P &= p_1 + p_2, \\ Q &= p_1 - p_2, \end{aligned} \tag{2.13}$$

and we denote by

$$M_{P,Q} = (\mathbf{w}, A_P) \tag{2.14}$$

one of the homogeneous Galilean transformations such that

$$\begin{aligned} p_1 &= M_{P,Q}\omega_1, \\ p_2 &= M_{P,Q}\omega_2. \end{aligned} \tag{2.15}$$

It follows that

$$\begin{aligned} P &= (\pi^0 + \mathbf{w}\cdot R(A_P)\boldsymbol{\pi}, R(A_P)\boldsymbol{\pi}), \\ Q &= (\chi^0 + m\mathbf{w}^2, 2m\mathbf{w}). \end{aligned} \tag{2.16}$$

Any member of the double coset under consideration can be written as $(M_{P,Q}L_1M_{\omega_1}, M_{P,Q}L_2M_{\omega_2})$ where $L_i \in G_{\omega_i}$ $(i = 1, 2)$. Therefore, by covariance,

$$f(M_{P,Q}L_1M_{\omega_1}, M_{P,Q}L_2M_{\omega_2}) = D^{s_1}(M_{\omega_1}^{-1}L_1M_{\omega_1}) D^{s_2}(M_{\omega_2}^{-1}L_2M_{\omega_2}) \times f(M_{P,Q}M_{\omega_1}, M_{P,Q}M_{\omega_2}). \tag{2.17}$$

If we put

$$f(M_{P,Q}LM_{\omega_1}, M_{P,Q}LM_{\omega_2}) = \tilde{f}(M_{P,Q}L), \tag{2.18}$$

the transformation law for $\tilde{f}(M_{P,Q})$ is

$$(U(a, M)\tilde{f})_{\sigma_1\sigma_2}(M_{P,Q}) = e^{iP\cdot a} D^{s_1}_{\sigma_1\tau_1}(M_{\omega_1}^{-1}M_{P,Q}^{-1}MM_{M_P^{-1}, M_Q^{-1}M_{\omega_1}}) \times D^{s_2}_{\sigma_2\tau_2}(M_{\omega_2}^{-1}M_{P,Q}^{-1}MM_{M_P^{-1}, M_Q^{-1}M_{\omega_2}}) \times \tilde{f}_{\tau_1\tau_2}(M_{M_P^{-1}, M_Q^{-1}}). \tag{2.19}$$

One can see that $M_{P,Q}^{-1}MM_{M_P^{-1}, M_Q^{-1}}$ belongs to $G_{\omega_1} \cap G_{\omega_2}$, which is the set of elements $(\mathbf{0}, A)$, such that $R(A)\mathbf{v} = \mathbf{v}$ and $\mathbf{v}$ is the same as in (2.10). Therefore, the M_{ω_i} $(i = 1, 2)$ which commute with $G_{\omega_1} \cap G_{\omega_2}$ can be dropped from the argument of D^{s_i} $(i = 1, 2)$ in (2.19). Furthermore, by quantizing both spins along $\mathbf{v}$ we can simultaneously diagonalize D^{s_1} and D^{s_2}. They take the form

$$D^{s_i}_{\sigma_i\tau_i}(M_{P,Q}^{-1}MM_{M_P^{-1}, M_Q^{-1}}) = \delta_{\sigma_i\tau_i} \exp\left[i\sigma_i\varphi(M_{P,Q}^{-1}MM_{M_P^{-1}, M_Q^{-1}})\right].$$

Looking at (2.14) one easily checks that

$$M_{P,Q} = M_P S_Q,$$

where

$$\begin{aligned} M_P &= (\mathbf{w}_1, A_P), \\ S_Q &= (R(A_P)^{-1}\mathbf{w}_2, 1), \end{aligned} \tag{2.20}$$

and $\mathbf{w}_1$, $\mathbf{w}_2$ are the components of $\mathbf{w}$ along $\mathbf{P}$ and in the plane orthogonal to $\mathbf{P}$, respectively. We recall that, according to (2.16),

$$\mathbf{w} = \mathbf{Q}/2m. \tag{2.21}$$

If $L \in G_{\omega_1} \cap G_{\omega_2}$, then $S_QL \in G_\pi$ and we can expand $\tilde{f}(M_{P,Q}L)$ according to (A4). One obtains

$$\tilde{f}_{\sigma_1\sigma_2}(M_PS_QL) = \frac{1}{2\pi}\sum_{-\infty}^{+\infty} e^{\frac{1}{2}il\varphi} \int d_2\mathbf{x} e^{-i\mathbf{x}\cdot R(A_P)^{-1}\mathbf{w}_2} \psi^{(l)}_{\sigma_1,\sigma_2}(\mathbf{x}, M_P), \tag{2.22}$$

where φ is the rotation corresponding to L.

By covariance [see (2.17)], it turns out that $l = \sigma_1 + \sigma_2$. Finally, it is straightforward to verify that the

$$e^{-i(\sigma_1+\sigma_2)\theta(C_\mathbf{x})}\psi^{(\sigma_1+\sigma_2)}_{\sigma_1,\sigma_2}(\mathbf{x}, M_P),$$

with $|\mathbf{x}| = r$ and $\epsilon = \pm 1$ according to whether $\sigma_1 + \sigma_2$ is an integer or a half-integer, transform

following (2.8). That is, the ψ are the basis for an irreducible unitary representation of zero mass.

3. COMPUTATION OF CLEBSCH-GORDAN COEFFICIENTS

As in Ref. 9 we introduce the state

$$|\phi\rangle = \int d_4p_1\, d_4p_2 \delta(2mp_1^0 - \mathbf{p}_1^2 - B_1) \times \delta(-2mp_2^0 - \mathbf{p}_2^2 - B_2) f_{\sigma_1\sigma_2}(M_{p_1}, M_{p_2}) \times |m, B_1, \mathbf{p}_1, s_1, \sigma_1\rangle\, |-m, B_2, \mathbf{p}_2, s_2, \sigma_2\rangle, \quad (3.1)$$

where $f_{\sigma_1\sigma_2}$ transform according to (2.9) and the $|m, B, \mathbf{p}, s, \sigma\rangle$ form a basis for an irreducible unitary representation of the Galilei group with mass $m \neq 0$, inner energy B, and spin s. We set the normalization to be

$$\langle m, B, \mathbf{p}, s, \sigma \,|\, m, B, \mathbf{p}', s, \sigma'\rangle = 2\,|m|\, \delta_3(\mathbf{p} - \mathbf{p}')\delta_{\sigma\sigma'}.$$

Since, clearly,

$$M_{P_1} = M_{P,Q} M_{\omega_1} N_1$$

and

$$M_{P_2} = M_{P,Q} M_{\omega_2} N_2,$$

with $N_i \in G_{h_i}$ $(i = 1, 2)$, we obtain by covariance

$$f_{\sigma_1\sigma_2}(M_{p_1}, M_{p_2}) = D^{s_1}_{\sigma_1\tau_1}(N_1^{-1}) D^{s_2}_{\sigma_2\tau_2}(N_2^{-1}) \tilde{f}_{\tau_1\tau_2}(M_{P,Q}),$$

where $\tilde{f}$ is given by (2.18).

After expanding $\tilde{f}_{\tau_1\tau_2}(M_{P,Q})$, as shown in (2.22), we substitute it in (3.1) and perform the change of variables (2.4). The result is

$$|\phi\rangle = \frac{1}{8\pi} \int_{-\infty}^{0} dB \int d_4P\, d_4Q \delta(\mathbf{P}^2 + B) \times \delta(4mQ^0 - \mathbf{Q}^2 + B - 2(B_1 + B_2)) \times \delta(2mP^0 - \mathbf{P}\cdot\mathbf{Q} + B_2 - B_1) \times D^{s_1}_{\sigma_1\tau_1}(N_1^{-1}) D^{s_2}_{\sigma_2\tau_2}(N_2^{-1}) \times \int d_2\mathbf{x} e^{-i\mathbf{x}\cdot R(A_P)^{-1}\mathbf{w}_2} \psi^{(\tau_1+\tau_2)}_{\tau_1,\tau_2}(\mathbf{x}, M_P) \times |m, B_1, \mathbf{p}_1, s_1, \sigma_1\rangle\, |-m, B_2, \mathbf{p}_2, s_2, \sigma_2\rangle. \quad (3.2)$$

One can rewrite (3.2) in the following way:

$$|\phi\rangle = \int_{-\infty}^{0} dB \int d_4P \delta(\mathbf{P}^2 + B) \int_0^\infty r\, dr \left(\frac{m}{4\,|\mathbf{P}|}\right)^{\frac{1}{2}} \times \int_0^{2\pi} d\theta \psi^{(\tau_1+\tau_2)}_{\tau_1,\tau_2}(r, \theta, M_P)\, |B, P, r, \theta; \tau_1, \tau_2\rangle, \quad (3.3)$$

where

$$|B, P, r, \theta, \tau_1, \tau_2\rangle = \frac{1}{4\pi}\left(\frac{|\mathbf{P}|}{m}\right)^{\frac{1}{2}} \int d_4Q \delta(4mQ^0 - \mathbf{Q}^2 + B - 2(B_1 + B_2)) \times \delta(2mP^0 - \mathbf{P}\cdot\mathbf{Q} + B_2 - B_1) \times D^{s_1}_{\sigma_1\tau_1}(N_1^{-1}) D^{s_2}_{\sigma_2\tau_2}(N_2^{-1}) e^{-iR(A_P)\mathbf{x}\cdot\mathbf{w}_2} \times |m, B_1, \mathbf{p}_1, s_1, \sigma_1\rangle\, |-m, B_2, \mathbf{p}_2, s_2, \sigma_2\rangle. \quad (3.4)$$

As ψ transform according to an irreducible unitary representation of zero mass, (3.4) form a basis for an irreducible unitary representation with zero mass, inner energy B, and degeneracy parameters τ_1 and τ_2. The normalization is given by

$$\langle B, P, r, \theta, \tau_1, \tau_2 \,|\, B', P', r', \theta', \tau_1', \tau_2'\rangle = \delta_{\tau_1\tau_1'}\delta_{\tau_2\tau_2'}\delta_4(P - P')\delta_2(R(A_P)(\mathbf{x} - \mathbf{x}')).$$

It is now straightforward to compute the Clebsch-Gordan coefficients, obtaining

$$\langle m, B_1, \mathbf{p}_1, s_1, \sigma_1; -m, B_2, \mathbf{p}_2, s_2, \sigma_2 \,|\, B, P, r, \theta, \tau_1, \tau_2\rangle = (2/\pi)(m\,|\mathbf{P}|)^{\frac{1}{2}} D^{s_1}_{\sigma_1\tau_1}(N_1^{-1}) D^{s_2}_{\sigma_2\tau_2}(N_2^{-1}) \times e^{-iR(A_P)\mathbf{x}\cdot\mathbf{w}_2} \delta_3(\mathbf{P} - \mathbf{p}_1 - \mathbf{p}_2) \times \delta(2mP^0 - \mathbf{P}\cdot(\mathbf{p}_1 - \mathbf{p}_2) + B_2 - B_1). \quad (3.5)$$

As expected, they satisfy the completeness property

$$\int d_4P\, d_2(R(A_P)\mathbf{x}) \sum_{-s_1}^{s_1} \sum_{-s_2}^{s_2} \times \langle m, B_1, \mathbf{p}_1, s_1, \sigma_1; -m, B_2, \mathbf{p}_2, s_2, \sigma_2 \,|\, B, P, r, \theta, \tau_1, \tau_2\rangle \times \langle B, P, r, \theta, \tau_1, \tau_2 \,|\, m, B_1, \mathbf{p}_1', s_1, \sigma_1'; -m, B_2, \mathbf{p}_2', s_2, \sigma_2'\rangle = 4m^2\delta_{\sigma_1\sigma_1'}\delta_{\sigma_2\sigma_2'}\delta_3(\mathbf{p}_1 - \mathbf{p}_1')\delta_3(\mathbf{p}_2 - \mathbf{p}_2'). \quad (3.6)$$

4. PARTIAL-WAVE ANALYSIS OF THE TWO-BODY SCATTERING AMPLITUDE IN THE CROSSED CHANNEL

In order to simplify the presentation we restrict ourselves in what follows to the problem of the elastic scattering of two spinless particles with zero internal energy and masses m_1 and m_2. We will denote by k_i and p_i, respectively, the incoming and outgoing four-momenta of the particle with mass m_i $(i = 1, 2)$.

The scattering matrix $S(\mathbf{p}_1, \mathbf{p}_2, \mathbf{k}_1, \mathbf{k}_2)$ is invariant under simultaneous Galilean transformations on the four particles. As discussed in Ref. 2, one must use for the outgoing particles the complex-conjugate representations. In our case this is equivalent to exchanging the mass m_i with the mass $-m_i$ and the four-momenta p_i with $-p_i$. We then decompose into irreducible representations the tensor product of the representation $|\mathbf{k}_i\rangle$ with the complex conjugate of the representation of $|\mathbf{p}_i\rangle$. This is nothing else but the decomposition performed in Sec. 2. Using the identity

$$S(\mathbf{p}_1, \mathbf{p}_2, \mathbf{k}_1, \mathbf{k}_2) = \int d_3\mathbf{p}_1'\, d_3\mathbf{p}_2'\, d_3\mathbf{k}_1'\, d_3\mathbf{k}_2' \delta_3(\mathbf{p}_1 - \mathbf{p}_1')\delta_3(\mathbf{p}_2 - \mathbf{p}_2') \times \delta_3(\mathbf{k}_1 - \mathbf{k}_1')\delta_3(\mathbf{k}_2 - \mathbf{k}_2') S(\mathbf{p}_1', \mathbf{p}_2', \mathbf{k}_1', \mathbf{k}_2')$$

and the completeness relation (3.6), one can write

$$S(\mathbf{p}_1, \mathbf{p}_2, \mathbf{k}_1, \mathbf{k}_2) = \int d_4P\, d_4P'\, d_2(R(A_P)\mathbf{x})\, d_2(R(A_P)\mathbf{x}') \times \langle m_1, \mathbf{p}_1; -m_1, -\mathbf{k}_1 \mid P\mathbf{x}\rangle \Gamma(P, P', \mathbf{x}, \mathbf{x}') \times \langle P'\mathbf{x}' \mid -m_2, -\mathbf{p}_2; m_2, \mathbf{k}_2\rangle, \quad (4.1)$$

where Γ is given by:

$$\Gamma(P, P', \mathbf{x}, \mathbf{x}') = (16m_1m_2)^{-2} \int d_3\mathbf{p}_1'\, d_3\mathbf{p}_2'\, d_3\mathbf{k}_1'\, d_3\mathbf{k}_2' \times \langle P\mathbf{x} \mid m_1, \mathbf{p}_1'; -m_1, -\mathbf{k}_1'\rangle S(\mathbf{p}_1', \mathbf{p}_2', \mathbf{k}_1', \mathbf{k}_2') \times \langle -m_2, -\mathbf{p}_2'; m_2, \mathbf{k}_2' \mid P'\mathbf{x}'\rangle. \quad (4.2)$$

Because S is Galilean-invariant, the distribution Γ is diagonal in P and $R(A_P)\mathbf{x}$. We write it as

$$\Gamma(P, P', \mathbf{x}, \mathbf{x}') = (\pi^2/4\,|\mathbf{P}|)(m_1m_2)^{-\frac{1}{2}}\delta_4(P - P') \delta_2(R(A_P)\mathbf{x} - R(A_{P'})\mathbf{x}')\gamma(P, R(A_P)\mathbf{x}). \quad (4.3)$$

Furthermore, $\gamma(P, R(A_P)\mathbf{x})$ is invariant under Galilean transformations which rotate $R(A_P)\mathbf{x}$ in the two-dimensional plane orthogonal to $\mathbf{P}$ and transform P following (2.4) with zero mass. As usual, we consider γ as a function of the invariants which are only $\mathbf{P}^2$ and $|\mathbf{x}|$, since $\mathbf{P} \cdot R(A_P)\mathbf{x} = 0$. Accordingly, the partial-wave expansion (4.1) takes the form

$$S(\mathbf{p}_1, \mathbf{p}_2, \mathbf{k}_1, \mathbf{k}_2) = \frac{1}{4m_1m_2}\delta\left(\frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} - \frac{\mathbf{k}_1^2}{2m_1} - \frac{\mathbf{k}_2^2}{2m_2}\right) \times \delta_3(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{k}_1 - \mathbf{k}_2)\int d_2\mathbf{y}\, e^{i\mathbf{y}\cdot\Delta}\gamma((\mathbf{p}_1 - \mathbf{k}_1)^2, |\mathbf{y}|), \quad (4.4)$$

where

$$\Delta = \frac{\mathbf{p}_1 + \mathbf{k}_1}{2m_1} - \frac{\mathbf{p}_2 + \mathbf{k}_2}{2m_2} \quad (4.5)$$

and the integration on $\mathbf{y}$ is performed in the plane orthogonal to $\mathbf{p}_2 - \mathbf{k}_2$. By going to polar coordinates, (4.4) becomes

$$S(\mathbf{p}_1, \mathbf{p}_2, \mathbf{k}_1, \mathbf{k}_2) = \frac{\pi}{2m_1m_2}\delta\left(\frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} - \frac{\mathbf{k}_1^2}{2m_1} - \frac{\mathbf{k}_2^2}{2m_2}\right) \times \delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{k}_1 - \mathbf{k}_2) \times \int_0^\infty r\, dr\gamma((\mathbf{p}_1 - \mathbf{k}_1)^2, r)J_0(r\,|\Delta|), \quad (4.6)$$

where J_0 is the Bessel function of zero order.

The important fact to be observed about either (4.4) or (4.6) is that γ depends on the momenta of the particles only through the momentum transfer $t = (\mathbf{p}_1 - \mathbf{k}_1)^2$. This makes these formulas particularly appropriate to study the high-energy behavior of the scattering amplitude at fixed-momentum transfer. In a relativistic theory, the corresponding property is that the "residue functions" depend only on t.

It is known that, if the potential is regular enough, the high-energy behavior of the scattering amplitude at fixed t is given by the Born term.[10] One can verify that, up to a constant, the corresponding γ^B is

$$\gamma^B(P, R(A_P)\mathbf{x}) = \delta_2(R(A_P)\mathbf{x})\tilde{V}(\mathbf{P}), \quad (4.7)$$

where $\tilde{V}$ is the Fourier transform of the potential. [If one wants to insert (4.7) into (4.6) the $\delta_2(R(A_P)\mathbf{x})$ has to be replaced by $-\delta'(r)$.] In this case, the high-energy behavior at fixed momentum transfer is given by a pole at the origin. The behavior of the other terms in the Born series is determined by the regularity of the corresponding γ terms in the r variable.

5. CONTRACTION OF THE POINCARÉ GROUP

Since the Galilei group is a contraction of the Poincaré group,[11] we will show that it is possible to reach (4.7) from the corresponding formula of the relativistic case [see formula (9) of Ref. 1]:

$$M(s, t, \mu^2) = 2\int_0^\infty \sigma\, d\sigma N(t, \sigma, \mu^2)P_{-\frac{1}{2}+i\sigma}\left(1 + \frac{2u}{t - 4\mu^2}\right), \quad (5.1)$$

where

$$s + t + u = 4\mu^2$$

by choosing a suitable limiting process. First we recall some machinery given in Ref. 11. If P_μ and $M_{\mu\nu}$ denote the usual generators of the Poincaré group, the Lie algebra of the Galilei group is obtained by multiplying P_k and M_{0k} by ϵ and letting ϵ tend to zero. As far as the irreducible unitary representations of the Poincaré group are concerned, if $m^2 > 0$ one obtains the corresponding representations of the Galilei group by taking $m^2 \sim \epsilon^{-4}$, whereas if $m^2 < 0$ one takes $m^2 \sim \epsilon^{-2}$.

Formula (5.1) is a partial-wave expansion performed by using the little group of a spacelike vector, that is $O(2, 1)$. Its Lie algebra is generated by M_{01}, M_{02}, M_{12}. In the representations appearing in (5.1), the eigenvalues of the Casimir operator $M_{12}^2 - M_{01}^2 - M_{02}^2$ are given by $-(\sigma^2 + \frac{1}{4})$. Since, in the contraction, ϵM_{0k} is chosen to have a limit as $\epsilon \to 0$, it follows that σ must behave like ϵ^{-1}. Therefore, in order to contract

[10] A. Klein and C. Zemach, Ann. Phys. (N.Y.) 7, 440 (1959).

[11] E. Inönü and E. P. Wigner, Proc. Natl. Acad. Sci. (US) 39, 510 (1953).

(5.1), one has to consider

$$\lim_{\epsilon\to 0} P_{-\frac{1}{2}+i(\lambda/\epsilon)}\left(1+\frac{2u\epsilon^2}{\epsilon^2 t-4\mu^2}\right)$$

which is equal to[12]

$$J_0\left(\lambda\frac{|\mathbf{p}_1-\mathbf{k}_2|}{\mu}\right).$$

We remark that in this limit only the space components survive in u. As a result, we see that in the nonrelativistic limit (5.1) reduces to (4.6), interpreting λ as r.

6. CONCLUSIONS

By partial-wave analysis in the crossed channel we have obtained a new parametrization of the two-body elastic scattering matrix in the nonrelativistic case. Our results show that, in the same way as in relativistic scattering, the partial-wave analysis in the t channel is connected to the high-energy behavior in the direct channel for fixed t. It is interesting to note, however, that, for amplitudes tempered in the momenta, the high-energy behavior is given only by what corresponds to the background term in the relativistic theory.

Finally it may turn out that the representation we have derived is a useful tool to study potential scattering, for example, by inserting it into the Lippmann–Schwinger equation.

ACKNOWLEDGMENT

Both the authors thank very much Professor B. Zumino for his kind hospitality at the Department of Physics of New York University.

APPENDIX

For the sake of completeness we classify here the irreducible unitary representations of the two-sheeted covering group in two dimension E_2.

We denote the generic element of E_2 by $(\mathbf{u}, C)$, where $\mathbf{u}$ is a two-dimensional translation and C an element of SU_2 which corresponds to a one-dimensional rotation. The product law is

$$(\mathbf{u}_1, C_1)(\mathbf{u}_2, C_2) = (\mathbf{u}_1 + R(C_1)\mathbf{u}_2, C_1C_2), \quad \text{(A1)}$$

where $R(C)$ is the rotation corresponding to C.

Still following Mackey,[6] we associate to each vector $\mathbf{x}$ a $C_\mathbf{x}$ such that $R(C_\mathbf{x})\mathbf{x}_0 = \mathbf{x}$, where $\mathbf{x}_0$ is a fixed vector on the orbit of $\mathbf{x}$, and we denote by θ the angle between $\mathbf{x}$ and $\mathbf{x}_0$. Then the infinite-dimensional irreducible unitary representations, labeled by $|\mathbf{x}| = r$ and $\epsilon = \pm 1$, are of the form

$$(U^{r,\epsilon}(\mathbf{u}, C)f)(C_\mathbf{x}) = e^{i\mathbf{u}\cdot\mathbf{x}} D^\epsilon(C_\mathbf{x}^{-1}CC_{C^{-1}\mathbf{x}})f(C_{C^{-1}\mathbf{x}}). \quad \text{(A2)}$$

$D^\pm$ is an irreducible unitary representation of the little group of $\mathbf{x}_0$ which is simply the group of two elements $\{1, -1\}$. The functions $f(C_\mathbf{x})$, at fixed r, must be considered L^2 functions with respect to the measure $d\theta$. The finite-dimensional representations are one dimensional and they are labeled by an integer or a half-integer

$$U(\mathbf{u}, C)f = e^{in\varphi}f,$$

where φ is the angle of rotation corresponding to C. The matrix elements of the infinite-dimensional representations are

$$\langle\theta|\, U^{r,+}(\mathbf{u}, C)\,|\theta'\rangle = \delta_{2\pi}(\theta' + \varphi - \theta)e^{i\mathbf{x}\cdot\mathbf{u}}, \quad \text{(A3)}$$

whereas those corresponding to $U^{r,-}$ differ from the ones above at most by a sign. $\delta_{2\pi}$ is the Dirac δ of period 2π. From (A3) it is clear that any function on the group $\in L^2$ can be expanded into the matrix elements of the infinite-dimensional irreducible unitary representations. More generally any tempered distribution has this expansion, since this amounts to performing a Fourier transform in $\mathbf{u}$. Explicitly, the expansion has the form

$$f(\mathbf{u}, C) = \frac{1}{2\pi}\sum_{-\infty}^{+\infty}{}_m\, e^{\frac{1}{2}im\varphi}\int d_2\mathbf{x}\, d_m(\mathbf{x})e^{-i\mathbf{x}\cdot\mathbf{u}}. \quad \text{(A4)}$$

If f is a tempered distribution, (A4) automatically includes the finite-dimensional representations which correspond to $d_m(\mathbf{x})$ concentrated at the origin.

[12] This formula can be obtained in the same way as the analogous ones in G.N. Watson, *Theory of Bessel Functions* (Cambridge University Press, Cambridge, England, 1958), p. 156.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

Critical Point Behavior of the Ising Model with Higher-Neighbor Interactions Present

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The method of developing exact power-series expansions for the partition function Z_N and related thermodynamic functions for the Ising model valid below the critical point is generalized to include exchange interactions between first-, second-, and third-neighbor pairs. Expansions of the spontaneous magnetization $M_0(T)$ and zero field susceptibility $\chi_0(T)$ are derived through to sixth order of perturbation for the s.q. lattice, and through to fifth order of perturbation for the Δ'^{r}, b.c.c., s.c., and f.c.c. lattices, when interactions $J_1 S_i^z S_j^z$ and $J_2 S_k^z S_l^z$ are present between first- and second-neighbor spins, respectively (second-neighbor model). These expansions have also been obtained for the case where interactions of equal magnitude ($J_1 = J_2 = J_3$) are present between first-, second-, and third-neighbor pairs (third-equivalent-neighbor model); here expansions through to fifth order of perturbation are obtained for the s.q., Δ'^{r}, b.c.c., and s.c. lattices and through to fourth order for the f.c.c. lattice. The Padé approximant-procedure is employed to discuss the effects of an extended but finite range of interaction on the behavior of $M_0(T)$ and $\chi_0(T)$ for $T \to T_c^-$ as characterized by the critical exponents β and γ', respectively. For the second-equivalent-neighbor model lattices, it is found that $0.122 \leq \beta \leq 0.134$ in two dimensions, and that $0.308 \leq \beta \leq 0.328$ in three dimensions; from which it is concluded that β remains unchanged from its value in the nearest-neighbor model. The corresponding limits for γ' in three dimensions are $1.18 \leq \gamma' \leq 1.28$; from this and the results for the b.c.c. lattice in particular, it is concluded that γ' is probably $\frac{5}{4}$ and hence the transition in χ_0 is symmetrical about T_c ($\gamma' = \gamma$). A repetition of this analysis for the third-equivalent-neighbor model three-dimensional lattices shows a marked shift in the estimated range of β and γ'; the results are $0.345 \leq \beta \leq 0.365$, and $1.01 \leq \gamma' \leq 1.14$. In each of the above cases, the corresponding high-temperature ($T > T_c$) expansions of $\chi_0(T)$ obtained previously have been analyzed to yield estimates of the critical exponent γ. The over-all results and in particular the estimates of γ for the s.q. and b.c.c. lattices suggest that this index is unaffected by extending the range of interaction, and that if γ is a rational fraction then it is the same fraction for the n.n. model and second- and third-equivalent neighbor models. Finally the high-temperature expansions of Z_N in zero field, and of $\chi_0(T)$ for the second-neighbor model are used to examine the dependence of the critical temperature T_c, the critical energy $(E_\infty - E_c)/kT_c$, and the critical entropy $(S_\infty - S_c)/k$ on the relative strengths of J_1 and J_2 for values of J_2/J_1 in the range 0 to 1. It is found that the variation of the critical point is well represented by

$$T_c(\alpha) = T_c(0)[1 + m_1\alpha],$$

where $\alpha = J_2/J_1$ and lies in the range $0 \leq \alpha \leq 1$; and $T_c(0)$ is the critical temperature of the nearest-neighbor model. The values of m_1 are 0.61, 2.47, 0.84, 1.45, and 1.35 for the f.c.c., s.c., b.c.c., s.q., and Δ'^{r} lattices, respectively. All these calculations are compared with the corresponding results for the Heisenberg model.

I. INTRODUCTION

This is a paper about the Ising model of a ferromagnet in which the approximation usually adopted, of only including nearest neighbor (n.n.) interactions ($J_1 S_i^z S_j^z$), is relaxed and interactions ($J_2 S_k^z S_l^z$) between next nearest neighbors (n.n.n.) are added into the Hamiltonian. We also discuss the inclusion of third-neighbor interactions. The Hamiltonian for an Ising-model lattice assembly of N spins, generalized to include interactions between 1st, 2nd, $\cdots$, nth neighboring spins, may be put in the form

$$\mathcal{H} = -\sum_{r=1}^{n} 2J_r \sum_{\langle r \rangle} 4S_i^z S_j^z - mH \sum_{i=1}^{N} 2S_i^z. \qquad (1)$$

In Eq. (1), S_i^z is the spin variable associated with the ith lattice site, J_r is the exchange integral between rth neighbors, H is the external magnetic field, m is the magnetic moment on each site, and $\sum_{\langle r \rangle}$ denotes the summation over all pairs of rth neighbors.

Recent years have seen a resurgence of interest in the Ising model and, although an exact solution for the three-dimensional nearest neighbor assemblies is still lacking, very successful efforts have been made towards elucidating their equilibrium behavior. The importance of the Ising model lies in that it represents in semi-classical terms the simplest model of a strongly interacting many-body system and is particularly useful in formulating the short-range interactions which are responsible for a variety of cooperative effects, where attention is focused on the phenomena

which occur very near critical points. Present interest in the theory of phase transitions is centered mainly on seeking a physical basis for the obviously similar nature of critical-point behavior in apparently very different types of phase separations. In this the Ising model is very useful, since it can be adopted as a model for such different phenomena as order–disorder phenomena in binary alloys, liquid–vapor condensation, and ferromagnetic and antiferromagnetic ordering processes. The effects of extending the range of interaction beyond nearest neighbors on these phenomena has been largely neglected in the literature, and it is hoped that the present publication will help in filling this gap. The reader who is uninterested in methodological detail can find a review of the results that have been obtained in the paper, together with the main interpretative points, by skipping to Sec. IX.

The literature on the Ising model is extensively reviewed; for an introduction to the general mathematical problems of approximate theories, exact treatments, and asymptotic methods, reference should be made to reviews by Newell and Montroll,[1] Domb,[2] Montroll,[3] Brout,[4] and Baker.[5] General interpretive reviews of critical-point phenomena have been given by Kadanoff,[6] Fisher,[7] and Domb and Miedema.[8] A historical review has recently been compiled by Brush.[9] Previous work specifically concerned with extending the range of interaction has been done by Hill,[10] Guggenheim and McGlashan,[11] Rushbrooke and Ursell,[12] Domb and Potts,[13] Domb and Dalton,[14] Dalton,[15] Vaks, Larkin, and Ovchinnikov,[16] Baker,[17] Kac and Helfand,[18] Hiley and Joyce,[19] and Joyce.[20]

Hill considered the effects of n.n.n. interactions in monolayers on a simple quadratic lattice using the quasichemical approximation, and Guggenheim and McGlashan extended the work to a treatment of regular mixtures for the s.c. and b.c.c. lattices. Rushbrooke and Ursell considered some of the properties of one-dimensional assemblies with any finite range of interaction, and Domb and Potts included n.n.n. interactions in two-dimensional lattices by developing exact series expansions for the partition function below the critical point. Vaks *et al.* have recently obtained an exact solution for the zero-field partition function and magnetization of the s.q. lattice with one-half of the n.n.n. interaction present.

Domb and Dalton have considered the critical properties such as the critical point, critical energy, and critical entropy of the second and third equivalent neighbor Ising-model lattices (see below) and have given estimates of asymptotic behavior for large coordination numbers. Dalton has given the high temperature expansions of the zero-field partition function and zero-field susceptibility for the second neighbor model (see below), valid for general spin. Baker, and Kac and Helfand have considered infinitely long-range forces of the type $\gamma J e^{-\gamma r}$ for one- and two-dimensional lattices, and an Ising model with interactions of the type $1/r^{d+\sigma}$, where d is the dimensionality and $\sigma > 0$, has been discussed by Hiley and Joyce. Finally Joyce has given a treatment of the spherical model with $1/r^{d+\sigma}$ type interactions.

All the existing mathematical techniques which enable the two-dimensional n.n. lattices to be solved exactly in zero field fail on the introduction of n.n.n. interactions, where the lattices become nonplanar. Consequently, the problem is effectively elevated to the difficulty of the 3-dimensional n.n. assemblies, and it is of interest to obtain the effect of this on critical-point phenomena, where dimensionality is considered to be of such importance. At the present time, the only models where the effect of n.n.n. interactions can be traced exactly are the linear loop of N spins, and Fisher's two-dimensional superexchange model of an antiferromagnet.[21]

In this paper we discuss both two- and three-dimensional assemblies, and the mathematical approach is one of developing series expansions for the partition function and related thermodynamic functions in regions above and below the critical temperature. It has by now been amply demonstrated that in the absence of any exact treatments the series-expansion approach is the only method which is

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[21] M. E. Fisher, Proc. Roy. Soc. (London) **A254**, 66 (1959); **A256**, 502 (1960).

powerful enough to yield an accurate account of the critical region. The presentation here is in terms of the Ising ferromagnet with (1) as the Hamiltonian and $S = \frac{1}{2}$, but much of the material, such as the configurational data and the conclusions on critical-point behavior, can be carried over to other problems such as binary alloys, absorbed monolayers, antiferromagnets, and the lattice gas model of Yang and Lee.[22]

The success of the series-expansion approach depends entirely on being able to extrapolate the thermodynamic functions to their singularities, and this in turn depends on how quickly the terms in the series settle down to a steady behavior. Previous work by the authors[23] on similar expansions for the Heisenberg model has shown that in many cases the lattices of large coordination number possess expansions which appear to settle down more rapidly than those of smaller coordination numbers. By introducing higher-order interactions, we can effectively increase the coordination numbers by equating the magnitudes of all interactions present; this model is known as the equivalent neighbor model. Thus, for example, the f.c.c. lattice with first, second, and third equal neighbor interactions has a coordination number of 42 compared with 12 for the n.n. model. It can be hoped, therefore, that the expansions for the equivalent neighbor model lattices will very quickly settle down to a smooth behavior from which extrapolations to critical behavior can be made. There is, of course, no sound basis for assuming that the partition function is uniformly convergent in the range of interaction, and although initial irregularities in the expansion coefficients can be removed by extending the range of interaction, a more rapid convergence is not assured.

In this paper we extensively analyze the series expansions of the equivalent neighbor model. The notation for the equivalent neighbor model lattices is as follows: A lattice L with n equivalent neighbor interactions present is denoted by $L(1, 2, \cdots, n)$ and will be referred to as the "nth equivalent neighbor model." Where we specifically wish to discuss the effects of n.n.n. interactions we refer to "the second neighbor model." The techniques used in this paper in extrapolating the expansions are the ratio methods of Domb and Sykes,[24] and the Padé-approximant methods introduced to these problems by Baker.[5]

Considerable experimental interest is attached to studying the effects of longer-range interactions on the thermodynamic functions and critical parameters, since here the effects are often too large to be ignored when detailed comparisons between theory and experiment are made. This has been clearly demonstrated by several authors in the case of the Heisenberg model, which provides a more realistic basis for such comparisons in magnetic work. Of the experimental work where the Ising model seems to be the appropriate model, one may mention the cobalt tuton salts such as $CoK_2(SO_4)_2 \cdot 6H_2O$ discussed by Domb and Miedema,[8] and the recent work on $CoCs_3Cl_5$ and $CoCs_3Br_5$ by the Leiden group.[25,26] References to the recent work on fluids and binary alloys can be found in Fisher's review article.

The plan of the paper is as follows. In Sec. II the theory of obtaining the low-temperature ($T \leq T_c$) perturbation expansions of the partition function with up to nth neighbor interactions present is outlined, and the expansions for the second neighbor model are obtained up to the fifth order of approximation. These expansions are also obtained for the $L(1, 2)$, and $L(1, 2, 3)$ lattices. All the low-temperature expansions are collected together in Appendices A and B. In Sec. III some of the combinatorial problems associated with determining the low-temperature lattice constants for configurations on lattices with nonequivalent bonds are described. The lattice constants of all configurations up to 5 spins are listed in Appendix C for the $L(1, 2)$ and $L(1, 2, 3)$ lattices. Padé-approximant methods are employed to analyze the low-temperature expansion of the equivalent neighbor model lattices in Sec. IV. Of primary interest are the critical exponents β and γ' of the zero-field magnetization M_0, and zero-field susceptibility χ_0, respectively, and Padé-approximant techniques of previous authors are employed to find estimates of these exponents for the $L(1, 2)$ and $L(1, 2, 3)$ lattices.

The high-temperature expansions ($T > T_c$) of the zero-field partition function and zero-field susceptibility are recalled in Sec. V; and the corresponding coefficients for the second neighbor model lattices are given in general form in Appendix D. In Sec. VI the variation of the critical point with the strength of the n.n.n. interactions is discussed, and the results are compared with the corresponding behavior of the Heisenberg model 3-dimensional lattices. The high-temperature approach of χ_0 to the critical region is considered in Sec. VII for the second and third equivalent neighbor model series, and estimates of the critical exponent γ are given. Here both ratio

[22] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404, 410 (1952).
[23] N. W. Dalton and D. W. Wood, Phys. Rev. **138**, A779 (1965).
[24] C. Domb and M. F. Sykes, J. Math. Phys. **2**, 63 (1961).
[25] K. W. Mess, E. Lagendijk, D. A. Curtis, and W. J. Huiskamp, Physica **33**, 555 (1967).
[26] R. F. Wielinga, H. W. J. Blote, J. A. Roest, and W. J. Huiskamp, Physica **33**, 1234 (1967).

methods and Padé-approximant methods are used. Finally, in Sec. VIII the variation of the critical energy and entropy with the magnitude of the n.n.n. interactions is discussed; estimates of these parameters are given for the second neighbor model lattices; and compared with the corresponding values for the Heisenberg model.

II. LOW-TEMPERATURE EXPANSIONS

The problems discussed in this section are those related to obtaining a low-temperature ($T \leq T_c$) series expansion for the partition function Z_N of the Ising ferromagnet. The procedure which naturally suggests itself is one of factorizing out of the partition function the ground-state energy E_0, where all the spins are aligned parallel, and deriving the contributions to Z_N from perturbations on E_0 obtained by overturning successive numbers of spins. For the case in which only one exchange parameter J_1 (n.n.) is involved, this method has been considerably developed by Domb,[27] Sykes,[28] Domb and Hiley[29]; and Sykes, Essam, and Gaunt.[30] Previous consideration to extending the problem to include two exchange parameters J_1 and J_2 (n.n., and n.n.n. interactions) has been given by Domb and Potts[13] (for two-dimensional lattices) and by Sykes[28]; however, these authors did not proceed beyond the fourth order of perturbation (see below).

Consider an Ising-model assembly of N spins with (1) as the Hamiltonian. The partition function is given by

$$Z_N(H, K_1, K_2, \cdots, K_n) = \sum_{S_i^z=\pm\frac{1}{2}} \left[\prod_{r=1}^{n} \exp\left(K_r \sum_{\langle r\rangle} S_i^z S_j^z\right)\right] \exp\left(L \sum_{i=1}^{N} 2S_i^z\right), \quad (2)$$

where the first summation is over a total of 2^N spin configurations of the assembly, and

$$K_r = 2J_r/kT \quad \text{and} \quad L = mH/kT. \quad (3)$$

Consider now the excited states E_s, which can result from s overturned spins on the lattice; for a given s the levels E_s depend on the relative positions taken by the overturned spins. For example, if two of the s spins are rth neighbors to each other the contribution to E_s is reduced by $2J_r$, relative to that configuration where the two spins are separated beyond the largest interaction range (nth neighbors). In a configuration of s overturned spins, let there be b_r which are rth neighbors ($r = 1, 2, \cdots, n$), and let q_r be the total number of rth neighbors of any particular spin (the rth neighbor coordination number); then the total number of rth neighbor pairs is $Nq_r/2$ and the total number of antiparallel rth neighbor pairs is $sq_r - 2b_r$. The sum over rth neighbor pairs in (1) becomes

$$4 \sum_{\langle r\rangle} S_i^z S_j^z = \frac{N}{2} q_r - 2(sq_r - 2b_r), \quad (4)$$

and

$$2 \sum_{i=1}^{N} S_i^z = N - 2s. \quad (5)$$

Combining (2), (4), and (5), we obtain

$$Z_N = \left[\sum_s \left(\prod_{r=1}^{n} u_r^{q_r s/2 - b_r}\right)\mu^s\right]\left[\mu^{-N/2}\left(\prod_{r=1}^{n} u_r^{-Nq_r/8}\right)\right], \quad (6)$$

where $u_r = \exp(-4K_r)$, $\mu = \exp(-2L)$, and $\sum_s$ is the summation over all configurations of s overturned spins ($s = 1, 2, \cdots, N$). We can group the expansion (6) as a series in ascending powers of μ with coefficients which are polynomials in $u_1, u_2, \cdots, u_n$; hence we write

$$Z_N = \left\{\mu^{-N/2} \prod_{r=1}^{n} u_r^{-Nq_r/8}\right\} \Lambda_N(u_1, u_2, \cdots, u_n, \mu), \quad (7)$$

where

$$\Lambda_N(u_1, u_2, \cdots, u_n, \mu) = \sum_{s=0}^{N} f_s^N(u_1, u_2, \cdots, u_n)\mu^s \quad (8)$$

and the polynomials $f_s^N(u_1, u_2, \cdots, u_n)$ are of degree $\leq q_r s/2$ in u_r. Direct evaluation of these "low temperature" polynomials soon becomes impracticable for large s, all the more so with a large number of parameters u_r. With one parameter the labor becomes prohibitive for $s > 9$, and for two parameters the work is tedious at $s = 4$. We illustrate here the procedure for the second neighbor model (taking $u_1 = u$ and $u_2 = v$) by obtaining the first three polynomials for the f.c.c. lattice ($q_1 = 12, q_2 = 6$). The illustrations also serve to introduce the notation for the configurational data in Appendix B. All the spin configurations which are referred to explicitly below are listed in Fig. 1.

A spin configuration of s overturned spins is represented by a linear graph G of s points, where any spins connected by a n.n. lattice spacing are drawn as $C(2, 1)$ in Fig. 1, and those separated by a n.n.n. lattice spacing are represented by $C_1(2, 1)$. Spins which are not n.n. or n.n.n. are unconnected and represented by $S(2, 1)$. We use $[G]_N$ to denote the

[27] C. Domb, Proc. Roy. Soc. (London) **199A**, 199 (1949).
[28] M. F. Sykes, Thesis, Oxford University, 1956.
[29] C. Domb and B. J. Hiley, Proc. Roy. Soc. (London) **A268**, 506 (1962).
[30] M. F. Sykes, J. W. Essam, and D. S. Gaunt, J. Math. Phys. **6**, 283 (1965).

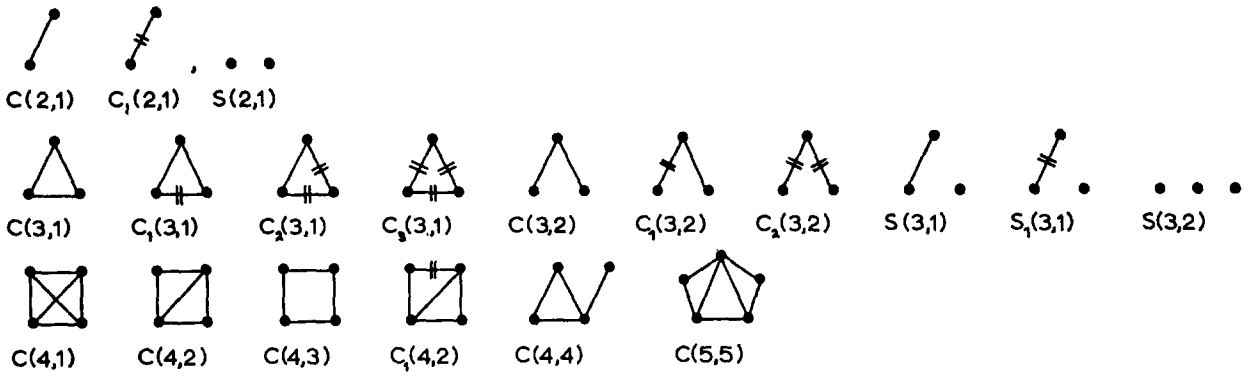

FIG. 1. The spin configurations which are referred to explicitly in Secs. 2 and 3. Here $C(x, y)$ and $S(x, y)$ are connected and separated configurations of x vertices and of topological type y respectively, and are examples of configurations occurring on a n.n. or an equivalent neighbor model lattice. The configurations $C_\alpha(x, y)$ or $S_\alpha(x, y)$ are examples of graphs occurring in the second neighbor model where α is the number of bonds connecting n.n.n. lattice points.

number of distinct separated graphs of type G, which can occur on a given lattice, and $N[G]$ denotes the number of connected graphs of type G. The low-temperature polynomials can be written in the form

$$f_s^N = \sum_{(G)} {}_s\,[G]_N W(G) + N \sum_{(G)} {}_s\,[G] W(G), \qquad (9)$$

where the first summation includes all separated graphs of s points, and the second summation includes all connected graphs of s points. The weight of each graph $W(G)$ is simply $u^{q_1 s/2 - b_1} v^{q_2 s/2 - b_2}$. Consider f_2^N; the only graphs for $s = 2$ are $[S(2, 1)]_N$, $N[C(2, 1)]$, and $N[C_1(2, 1)]$, thus

$$f_2^N = [S(2, 1)]_N u^{q_1} v^{q_2} + N[C(2, 1)] \times u^{q_1 - 1} v^{q_2} + N[C_1(2, 1)] u^{q_1} v^{q_2 - 1}. \qquad (10)$$

Continuing in this manner we obtain $f_3^N(u, v)$, which is

$$\begin{aligned} f_3^N = {} & [S(3, 2)]_N u^{3q_1/2} v^{3q_2/2} + [S(3, 1)]_N u^{3q_1/2 - 1} v^{3q_2/2} \\ & + [S_1(3, 1)]_N u^{3q_1/2} v^{3q_2/2 - 1} + N[C(3, 2)] \\ & \times u^{3q_1/2 - 2} v^{3q_2/2} + N[C_1(3, 2)] u^{3q_1/2 - 1} v^{3q_2/2 - 1} \\ & + N[C_2(3, 2)] u^{3q_1/2} v^{3q_2/2 - 2} + N[C(3, 1)] \\ & \times u^{3q_1/2 - 3} v^{3q_2/2} + N[C_1(3, 1)] u^{3q_1/2 - 2} v^{3q_2/2 - 1} \\ & + N[C_2(3, 1)] u^{3q_1/2 - 1} v^{3q_2/2 - 2} \\ & + N[C_3(3, 1)] u^{3q_1/2} v^{3q_2/2 - 3}. \end{aligned} \qquad (11)$$

Following Domb[2] we obtain the partition function per spin Z by putting $N = 1$ in (7) and (9), and $\log Z$ is equal to the coefficient of N in (7). In the expansion of Z, (8) is written in the form

$$\Lambda(u_1, u_2, \cdots, u_n, \mu) = \sum_{s=0}^{N} f_s(u_1, u_2, \cdots, u_n) \mu^s, \qquad (12)$$

and

$$\log \Lambda(u_1, u_2, \cdots, u_n, \mu) = \sum_{s=1}^{\infty} g_s(u_1, u_2, \cdots, u_n) \mu^s, \qquad (13)$$

where $f_s = f_s^{N=1}$, and g_s is the coefficient of N in f_s^N. The direct enumeration and counting of independent occurrences of the low-temperature configurations soon becomes complicated by the very rapid increase in the number of diagrams contributing to $f_s(u, v)$.

This problem can be partially overcome by employing the transformation between the low-temperature and high-temperature developments of the Ising model, which was discovered by Domb,[27] and subsequently developed by Wakefield[31] and Sykes.[28] In the case of the second neighbor model, the transformation is such that the expansion (12) can be written in the form

$$\sum_{s=0}^{\infty} f_s(u, v) \mu^s = \sum_{s+t=0}^{\infty} \varphi_{s,t}(\mu)(1 - u)^s (1 - v)^t / (1 + \mu)^{2(s+t)-1}, \qquad (14)$$

where

$$\varphi_{s,t}(\mu) = \sum_{\nu=0}^{2(s+t)} \alpha_\nu^{s,t} \mu^\nu \qquad (15)$$

and is a symmetric polynomial of degree $\leq 2(s + t)$ in μ. From (14) we readily obtain

$$\sum_{0}^{\infty} f_s^{p,q}(1, 1) \mu^s = (-1)^{p+q} p!\, q!\, \varphi_{p,q}(\mu) / (1 + \mu)^{2(p+q)-1}, \qquad (16)$$

where

$$f_s^{p,q}(1, 1) = \frac{\partial^{p+q}}{\partial u^p \partial v^q} f_s(u; v)\Big|_{\substack{u=1 \\ v=1}}. \qquad (17)$$

The symmetric polynomials (15) are known as the high-temperature polynomials, and the set of

$$\tfrac{1}{2}(n + 1)(n + 2)\, \varphi_{p,q}(\mu) \quad (p + q = t, t = 0, 1, 2, \cdots, n)$$

[31] A. J. Wakefield, Proc. Cambridge Phil. Soc. 47, 419 (1952).

can be obtained by equating the coefficients of μ^s in (16) and solving the resulting $\frac{1}{2}(n+1)(n+2)$ sets of s simultaneous equations

$$\mathbf{F}^{p,q} = \mathbf{A}^{p,q}\mathbf{a}^{p,q} \quad (p+q=s, s=0,1,2,\cdots,n), \tag{18}$$

where $F^{p,q}$ and $a^{p,q}$ are the column vectors

$$[f_0^{p,q}(1,1), f_1^{p,q}(1,1), \cdots, f_s^{p,q}(1,1)]$$

and

$$(\alpha_0^{p,q}, \alpha_1^{p,q}, \cdots, \alpha_s^{p,q}),$$

respectively, and $A^{p,q}$ is the matrix obtained on equating coefficients in (16). Since $\varphi_{p,q}(\mu)$ is a symmetric polynomial of degree $\leq 2(p+q)$, Eqs. (18) suffice to determine the polynomial completely.

Having determined the set of polynomials $\varphi_{p,q}(\mu)$ up to order $p+q=n$, we can use them to partially determine the low-temperature polynomial $f_{n+1}(u,v)$, where the part to be derived is arbitrary, and hence can be chosen to coincide with that part which is most difficult to evaluate directly; namely, the contribution from separated configurations. Using (16) and the $\frac{1}{2}(n+1)(n+2)$ polynomials $\varphi_{p,q}(\mu)$ $(p+q=n)$, we can obtain each of the $\frac{1}{2}(n+1)(n+2)$ partial derivatives $f_{n+1}^{p,q}(1,1)$ $(p+q=t, t=0,1,2,\cdots n)$; consequently, if all but $\frac{1}{2}(n+1)(n+2)$ of the coefficients in $f_{n+1}(u,v)$ are obtained by direct counting methods (see Sec. III), the remaining coefficients can be obtained by setting up a system of $\frac{1}{2}(n+1)(n+2)$ simultaneous equations. This implies that only the configuration of $s+1$ vertices and $\geq s+1$ lines need be enumerated directly. Thus we may write

$$f_{n+1}(u,v) = F_{n+1}(u,v) + G_{n+1}(u,v), \tag{19}$$

where $F_{n+1}(u,v)$ is obtained by direct counting and $G_{n+1}(u,v)$ contains $\frac{1}{2}(n+1)(n+2)$ unknown coefficients. The $\frac{1}{2}(n+1)(n+2)$ simultaneous equations are obtained from (19) by differentiating p times with respect to u and q times with respect to v, whence we obtain

$$G_{n+1}^{p,q}(1,1) = f_{n+1}^{p,q}(1,1) - F_{n+1}^{p,q}(1,1). \tag{20}$$

The solution of (20) completes the derivation of $f_{n+1}(u,v)$.

The technique is clearly illustrated by the following outline of the derivation of $f_3(u,v)$ for the f.c.c. lattice given in (11). Direct counting yields

$$\begin{aligned} f_1 &= u^6v^3, \\ f_2 &= 3u^{12}v^5 + 6u^{11}v^6 - 9u^{12}v^6, \end{aligned} \tag{21}$$

from which we obtain

$$\begin{aligned} &\varphi_{0,0} = 1, \quad \varphi_{1,0} = -6\mu, \quad \varphi_{0,1} = -3\mu, \\ &\varphi_{2,0} = 15\mu - 21\mu^2 + 15\mu^3, \\ &\varphi_{1,1} = 18\mu - 18\mu^2 + 18\mu^3, \\ &\varphi_{0,2} = 3\mu - 6\mu^2 + 3\mu^3. \end{aligned} \tag{22}$$

The only configurations contributing to $F_3(u,v)$ are

$$\begin{aligned} &N[C(3,1)] = 8N, \quad N[C_1(3,1)] = 12N, \\ &N[C_2(3,1)] = 0, \quad N[C_3(3,1)] = 0, \end{aligned}$$

which correspond to the terms $8u^{15}v^9$, $12u^{16}v^8$, $0u^{17}v^7$, and $0u^{15}v^6$ respectively in $f_3(u,v)$, which can now be represented in the matrix form

$$f_3(u,v) = \begin{array}{c|cccc} & u^{18} & u^{17} & u^{16} & u^{15} \\ & 0 & 1 & 2 & 3 \leftarrow \text{(n.n.)} \\ \hline v^9\ 0 & x_1 & x_2 & x_3 & 8 \\ v^8\ 1 & x_4 & x_5 & 12 & \\ v^7\ 2 & x_6 & 0 & & \\ v^6\ 3 & 0 & & & \\ \uparrow & & & & \\ \text{(n.n.n.)} & & & & \end{array} \tag{23}$$

$$\begin{aligned} = {} & x_1v^9u^{18} + x_2v^9u^{17} + x_3v^9u^{16} + x_4v^8u^{18} \\ & + x_5v^8u^{17} + x_6v^7u^{18} + 8v^9u^{15} + 12v^8u^{16}. \end{aligned} \tag{24}$$

Using (16) and (20)–(22), we can set up six simultaneous equations to obtain

$$\begin{aligned} f_3(u,v) = {} & 142v^9u^{18} - 162v^9u^{17} + 30v^9u^{16} - 93v^8u^{18} \\ & + 48v^8u^{17} + 15v^7u^{18} + 8v^9u^{15} + 12v^8u^{16}, \end{aligned} \tag{25}$$

from which we can derive the high-temperature polynomials $\varphi_{3,0}$, $\varphi_{1,2}$, $\varphi_{2,1}$, and $\varphi_{0,3}$, and continue the process for $f_4(u,v)$.

The technique above has been used to obtain the high-temperature and low-temperature polynomials for the second neighbor model up to the order of five overturned spins for the s.c., b.c.c., f.c.c., and triangular (Δ^r) lattices; for the s.q. lattice the polynomials up to sixth order have been derived. These polynomials are listed in Appendix A, where the low-temperature polynomials are given in the form $g_s(u,v)$ of Eq. (13), which is the form needed to derive the thermodynamic functions. By setting $u=v$ $(J_1=J_2)$, we obtain the low-temperature polynomials for the second equivalent neighbor model lattices with coordination number $q=q_1+q_2$. The calculations have also been done for the third equivalent neighbor model lattices $(J_1=J_2=J_3)$, where again the polynomials up to fifth order have been derived for the above lattices except in the case of the f.c.c. lattice,

where only the first four polynomials have been obtained. These results are tabulated in Appendix B.

III. ENUMERATIONS OF LOW-TEMPERATURE CONFIGURATIONS

A review of the techniques employed to obtain the lattice constants $N[G]$ and $[G]_N$ of both high-temperature and low-temperature configurations has been given by Domb.[2] The only new feature introduced into these techniques by the inclusion of second or higher neighbor interactions is the occurrence of the various types of nonequivalent bonds. For the low-temperature configurations above there is also the added restraint that no two spins, which are not connected by a bond, can be first, second, $\cdots$, or rth neighbors. For example, care is needed to ensure that all the space types (see below) of $C(4, 4)$ are not confused with $C_1(4, 2)$ when first and second neighbor interactions are present.

The most difficult configurations to count are those containing separated components; the extreme case at the nth order of approximation being the n separated spins. The symbolic method of Domb and Sykes,[2,28] where the separated configurations can be reduced in two stages to involve only the counting of multiply connected configurations, can be readily extended to include higher-order interactions. For example, with first and second neighbor interactions present, the symbolic equations for $[S(2, 1)]_N$ and $[S(3, 2)]_N$ become

$$[S(2, 1)]_N = N(N - 1)/2 - N(q_1 + q_2)/2, \quad (26)$$

and

$$\begin{aligned}[S(3, 2)]_N = {} & N(N - 1)(N - 2)/6 + N(q_1 + q_2) \\ & \times (q_1 + q_2 + 1 - N)/2 - N[C(3, 1)] \\ & - N[C_1(3, 1)] - N[C_2(3, 1)] \\ & - N[C_3(3, 1)], \end{aligned} \quad (27)$$

where the counting of three separated spins is reduced to the counting of the four possible triangles made up of first and second neighbor bonds. The effect of having two types of bond greatly increases the number of topologically distinct, multiply connected configurations, of which the lattice constants $N[G]$ must be determined directly by examining the lattice and using Wakefield's[31] method of space types. The number of space types of a given configuration is simply the number of orientations it can assume on the lattice, which are not related through rotational or translational symmetry. The contribution of each space type to $N[G]$ is the number of rotationally distinct orientations it can adopt on the lattice (see Fig. 1). Again the presence of two or more types of bond increases the number of space types of a given configuration.

If we ignore the finer details of longer-range interactions and successively include 1st, 2nd, $\cdots$, nth neighbor interactions of equal magnitude, we obtain the equivalent neighbor model, where all bonds are equivalent. The enumeration of configurations is now the same as for the n.n. model, and the counting of configurations is in effect the same as for the n.n. model with the lattice having a larger coordination number. As examples, we quote the following results for the f.c.c.(1), f.c.c.(1, 2) and f.c.c.(1, 2, 3) lattices.

$$\begin{aligned} &\text{f.c.c.(1)}, \quad q = 12, \quad && N[C(3, 1)] = 8N, \\ &\qquad N[C(4, 3)] = 3N, && N[C(4, 2)] = 24N \\ &\qquad N[C(4, 1)] = 2N, \\ &\text{f.c.c.(1, 2)}, \quad q = 18, && N[C(3, 1)] = 20N, \\ &\qquad N[C(4, 3)] = 9N, && N[C(4, 2)] = 84N, \\ &\qquad N[C(4, 1)] = 17N, \\ &\text{f.c.c.(1, 2, 3)}, \quad q = 42, && N[C(3, 1)] = 124N, \\ &\qquad N[C(4, 3)] = 105N, && N[C(4, 2)] = 1320N, \\ &\qquad N[C(4, 1)] = 333N. \end{aligned} \quad (28)$$

In Fig. 2 we list the different space types of the configuration $C(5, 5)$, containing first and second neighbor bonds, which can occur on the b.c.c. lattice. The contributions of each space type to the lattice constant for the second equivalent neighbor model are shown in parenthesis, and we obtain

$$N[C(5, 5)] = 156N. \quad (29)$$

The configurational data relating to diagrams containing nonequivalent bonds is too extensive to be included here; consequently, in Appendix C we list only the lattice constants of the equivalent neighbor model configurations. All the configurations

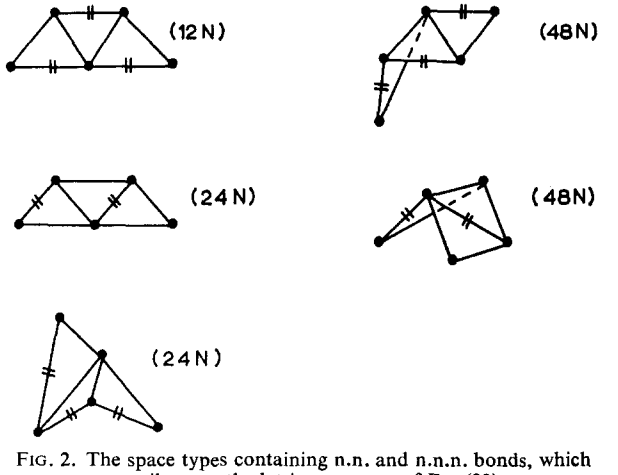

FIG. 2. The space types containing n.n. and n.n.n. bonds, which contribute to the lattice constant of Eq. (29).

of up to 5 separated spins are listed for the second and third equivalent neighbor model lattices except for the f.c.c.(1, 2, 3), where the configurations are only tabulated up to four spins.

IV. THE LOW-TEMPERATURE CRITICAL-POINT BEHAVIOR OF THE ZERO-FIELD MAGNETIZATION AND SUSCEPTIBILITY

From the low-temperature polynomials given in Appendices A and B, and the thermodynamic relations

$$M_0/Nm = 1 - 2\frac{\partial}{\partial\mu}\log\Lambda(u, v, \mu)|_{\mu=1} \qquad (30)$$

and

$$kT\chi_0/4Nm^2 = \bar{\chi}_0 = \frac{\partial}{\partial\mu}\log\Lambda(u,v,\mu)|_{\mu=1} + \frac{\partial^2}{\partial\mu^2}\log\Lambda(u,v,\mu)|_{\mu=1}, \qquad (31)$$

we can construct the low-temperature ($T < T_c$) series expansions for the zero-field magnetization M_0 and susceptibility χ_0. Our purpose here is to examine in detail the critical-point behavior ($T \to T_c^-$) of these two functions. We are primarily interested in the detection of any effects of extending the range of interaction on the behavior near the critical point. For this purpose we have elected to examine the equivalent neighbor model lattices, since it is to be expected that the finer details of the extended range (relative strengths) will be no more significant than their existence. The lattices which we have examined are the two- and three-dimensional second equivalent neighbor model lattices, and the b.c.c.(1, 2, 3) and s.c.(1, 2, 3) lattices. The expansions of M_0 and $\bar{\chi}_0$ for these lattices are given in Tables I, II, and III.

TABLE I. The zero-field magnetization series for the $L(1, 2)$ lattices, $M_0 = 1 - 2u^{q/2} + u^{q-1}\sum_{n=0}^{\infty} a_n u^n$.

n	f.c.c.(1, 2) $q = 18$ a_n	s.c.(1, 2) $q = 18$ a_n	b.c.c.(1, 2) $q = 14$ a_n	$\Delta(1, 2)$ $q = 12$ a_n	s.q.(1, 2) $q = 8$ a_n
0	−36	−36	−28	−24	−16
1	38	38	30	26	18
2	0	0	0	0	−24
3	0	0	0	0	−104
4	0	0	0	−60	248
5	0	0	−72	−216	−516
6	0	0	−330	+684	−328
7	−120	−120	960	−450	+2292
8	−558	−558	−560	−264	−7200
9	1584	1584	−48	−888	+4676
10	−908	−908	−336	−216	+14120
11	0	0	−1560	10602	
12	0	0	−1240	−18360	
13	−136	−104	19980	3354	
14	−672	−768	−28980	−3528	
15	−3432	−3432	8926	+29064	
16	−3208	−2888	−7296	+93900	
17	43908	43428	−13128		
18	−60564	−60216	54028		
19	23806	23542	271032		
20	−2310	−1530	−882804		
21	−6720	−7800			
22	−18532	−21760			
23	−43800	−36720			
24	146370	155370			
25	822848	785660			
26	−2445144	−2402604			
27	2187864	2163792			
28	−752650	−731476			

TABLE II. The low-temperature zero-field susceptibility series for the $L(1, 2)$ lattices, $\chi_0 = u^{q/2}\{1 + \sum_{n=1}^{\infty} h_n u^n\}$.

n	f.c.c.(1, 2) $q = 18$ h_n	s.c.(1, 2) $q = 18$ h_n	b.c.c.(1, 2) $q = 14$ h_n	$\Delta(1, 2)$ $q = 12$ h_n	s.q.(1, 2) $q = 8$ h_n
1	0	0	0	0	0
2	0	0	0	0	0
3	0	0	0	0	16
4	0	0	0	0	−18
5	0	0	0	24	36
6	0	0	28	−26	160
7	0	0	−30	0	−340
8	36	36	0	0	980
9	−38	−38	0	90	808
10	0	0	0	324	−3802
11	0	0	108	−1026	16464
12	0	0	495	695	−7175
13	0	0	−1440	528	−25864
14	0	0	840	1776	
15	180	180	96	492	
16	837	837	672	−21009	
17	−2376	−2376	3120	37572	
18	1362	1362	2480	−4714	
19	0	0	−39900	9414	
20	0	0	58230	−70128	
21	272	208	−16552	−230418	
22	1344	1536	18258		
23	6864	6864	32964		
24	6416	5776	−134134		
25	−87816	−86856	−674556		
26	121158	120432	2216310		
27	−47492	−46864			
28	5775	3825			
29	16800	19500			
30	46336	54400			
31	109500	91800			
32	−365745	−388245			
33	−2055824	−1963400			
34	6115812	6010182			
35	−5456592	−5395656			
36	1920365	1859080			

A slight extension of the configurational data in Appendix C is required to obtain the expansions in Tables I and II. First a small number of the lower-order terms in $g_{n+1}(u, v)$ may contribute to the same order of approximation as the higher-order terms in $g_n(u, v)$ on setting the field equal to zero ($\mu = 1$). These "overlap" contributions arise from the most closely packed configurations in $g_{n+1}(u, v)$ and can be enumerated without much difficulty. On the other hand we can use this effect to advantage by partially evaluating $f_{n+1}(u, v)$ and extending the series expansions. For example, the polynomials $g_1(u, v)$ to $g_5(u, v)$ yield the series of $M_0(u)$ on the b.c.c.(1, 2) lattice correct through to terms in u^{28}. The initial terms in

TABLE III. The series expansions of M_0 and χ_0 for the b.c.c.-(1, 2, 3) and s.c.(1, 2, 3) lattices (see Tables I and II for the notation).

M_0 n	b.c.c.(1, 2, 3) $q = 26$ a_n	s.c.(1, 2, 3) $q = 26$ a_n	b.c.c.(1, 2, 3) $q = 26$ h_n	s.c.(1, 2, 3) $q = 26$ h_n	χ_0 n
0	−52	−52	0	0	1
			⋮	⋮	⋮
1	54	54	0	0	11
2	0	0	52	52	12
	⋮	⋮			
10	0	0	−54	−54	13
11	−264	−264	0	0	14
			⋮	⋮	⋮
12	−1158	−1158	396	396	23
13	3264	3264	1737	1737	24
14	−1844	−1844	−4896	−4896	25
15	0	0	2766	2766	26
	⋮	⋮			
20	0	0	0	0	27
			⋮	⋮	⋮
21	−456	−536	0	0	32
22	−2304	−2304	912	1072	33
23	−10824	−10104	4608	4608	34
24	−8232	−9512	21648	20208	35
25	129972	130692	16464	19024	36
26	−178008	−178008	−259944	−261384	37
27	69854	69774	356016	356016	38
28	0	0	−139708	−139548	39
29	0	0	0	0	40
30	−280	−560	0	0	41
31	−2360	−1920	700	1400	42
32	−8670	−12510	5900	4800	43
33	−38440	−32920	21675	31275	44
34	−87320	−81120	96100	82300	45
35	−180000	−159120	218300	202800	46
36	713670	600030	450000	397800	47
37	3421240	3561480	−1784175	−1500075	48
			−8553100	−8903700	49

$f_6(u, v)$ are obtained from configurations of six spins and 15, 14, 13, ... lines; for the b.c.c.(1, 2) lattice there are no six spin figures with 15 or 14 lines and only one of 13 lines, which contributes the term $3u^{29}$ to $f_6(u, v)$. By enumerating the configurations of six spins and nine or more lines, and those of seven spins and 16 lines, the series for M_0 may be extended to terms in u^{33} as recorded in Table I. Similar considerations apply to the other series in Tables I and II.

The series expansions of M_0 and $\bar{\chi}_0$ for the n.n. model three-dimensional lattices have been examined by Baker,[32] Essam and Fisher,[33] Gaunt *et al.*,[34] and Baker and Gaunt.[35] Interest lies in seeking the critical point $u_c[= \exp(-4J/kT_c)]$ and the critical point exponents[36] β and γ', where

$$M_0(T) \sim D(T_c - T)^{\beta}|_{T \to T_c^-} \tag{32}$$

and

$$\bar{\chi}_0(T) \sim C(T_c - T)^{-\gamma'}|_{T \to T_c^-}. \tag{33}$$

In (32) and (33), D and C are the amplitudes of the singularities at $T = T_c$; they represent slowly varying functions of temperature in the critical region. Using three basic Padé-approximant techniques[37] (also employed by ourselves below) the latest figures for β and γ' are given by Baker and Gaunt as

$$\beta = 0.312 \begin{matrix} +0.003 \\ -0.006 \end{matrix} \simeq \tfrac{5}{16} \tag{34}$$

and

$$\gamma' = 1.310 \begin{matrix} +0.030 \\ -0.050 \end{matrix} \simeq 1\tfrac{5}{16}. \tag{35}$$

In establishing these results Baker and Gaunt considered the low-temperature specific-heat exponent α', and the critical-isotherm exponent δ, and then employed the rigorous inequalities of Rushbrooke[38] and Griffiths.[39]

We have analyzed the low-temperature series in Tables I, II, and III using Padé approximants and have employed the devices of Baker,[32] and Essam and Fisher.[33] First we have calculated some of the approximants for the series

$$\frac{d}{du} \log M_0(u) \sim \beta/(u - u_c) + \frac{d}{du} \log D(u)|_{u \to u_c^-} \tag{36}$$

and

$$\frac{d}{du} \log \bar{\chi}_0 \sim -\gamma'/(u - u_c) + \frac{d}{du} \log C(u)|_{u \to u_c^-}. \tag{37}$$

By selecting the appropriate poles of the approximants, and their corresponding residues, we obtain a sequence of estimates for u_c, β, and γ'. The results of these calculations for the second equivalent neighbor model lattices are shown in Tables IV and V; the corresponding results for the b.c.c.(1, 2, 3) and s.c.(1, 2, 3) lattices are given in Table VI. The estimates contained in these Tables, and in all subsequent tables of this section, have been obtained from the sequence of $[N, N]$ and $[N, N \pm 1]$ approximants.[40] Although the present series are longer than the corresponding n.n. series considered by Baker and Gaunt, we should not anticipate any greater accuracy in the results at this stage. The rate of convergence of the series appears

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[35] G. A. Baker, Jr. and D. S. Gaunt, Phys. Rev. **155**, 545 (1967).
[36] See Fisher's review for the notation on critical exponents.
[37] See Refs. 5 and 33.
[38] G. S. Rushbrooke, J. Chem. Phys. **39**, 842 (1963).
[39] R. B. Griffiths, Phys. Rev. Letters **14**, 623 (1965).
[40] The notation for the $[N, M]$ approximant is the same as employed by Fisher in Ref. 7.

TABLE IV. Padé approximant estimates of the critical temperatures u_c and the critical exponents γ' and β from $d/du \log M_0(u)$ and $d/du \log \chi_0(u)$ for the three-dimensional lattices with two equivalent neighbor interactions.

f.c.c.(1, 2)						s.c.(1, 2)						b.c.c.(1, 2)					
[M, N]						[M, N]						[M, N]					
M_0	χ_0	u_c from M_0	u_c from χ_0	β	γ'	M_0	χ_0	u_c from M_0	u_c from χ_0	β	γ'	M_0	χ_0	u_c from M_0	u_c from χ_0	β	γ'
16, 16	11, 11	0.7743	0.7971	0.3499	1.5651	16, 16	11, 11	0.7745	0.7975	0.3521	1.5699	10, 10	6, 6	0.7023	0.7351	0.2709	1.5684
16, 17	11, 12	0.7742	0.7971	0.3488	1.5649	16, 17	11, 12	0.7744	0.7964	0.3507	1.5553	10, 11	6, 7	...	0.7344	...	1.5577
17, 16	12, 11	0.7741	0.7971	0.3483	1.5649	17, 16	12, 11	0.7743	0.7959	0.3499	1.5464	11, 10	7, 6	0.7080	0.7338	0.3043	1.5481
17, 17	12, 12	0.7742	0.7971	0.3493	1.5651	17, 17	12, 12	0.7744	0.7972	0.3514	1.5664	11, 11	7, 7	0.7109	0.7351	0.3248	1.5687
17, 18	12, 13	0.7739	0.7754	0.3463	1.1898	17, 18	12, 13	...	0.7759	...	1.1976	11, 12	7, 8	0.7075	0.7464	0.2994	1.7262
18, 17	13, 12	0.7743	0.7994	0.3507	1.5932	18, 17	13, 12	0.7745	0.7792	0.3526	1.5914	12, 11	8, 7	0.7093	0.7367	0.3131	1.5887
18, 18	13, 13	0.7742	0.7771	0.3495	1.2249	18, 18	13, 13	0.7745	0.7776	0.3517	1.2304	12, 12	8, 8	0.7090	0.7334	0.3106	1.5483
18, 19	13, 14	0.7742	0.7766	0.3492	1.2152	18, 19	13, 14	0.7744	0.7772	0.3512	1.2210	12, 13	8, 9	0.7090	0.7036	0.3106	1.1240
19, 18	14, 13	0.7742	0.7764	0.3491	1.2112	19, 18	14, 13	0.7744	0.7769	0.3505	1.2168	13, 12	9, 8	0.7090	0.7385	0.3106	1.6061
19, 19	14, 14	0.7742	0.7772	0.3497	1.2266	19, 19	14, 14	0.7747	0.7776	0.3538	1.2318	13, 13	10, 10	0.7090	0.7093	0.3106	1.2136
19, 20	14, 15	0.7826	0.7753	0.3086	1.1874	19, 20	14, 15	0.7745	0.7759	0.3520	1.1955	13, 14	10, 11	0.7082	0.7069	0.3038	1.1708
20, 19	15, 14	0.7745	0.7641	0.3520	0.8980	20, 19	15, 14	0.7745	0.7622	0.3517	0.8407	14, 13	11, 10	0.7094	0.7002	0.3133	1.0266
20, 20	15, 15	0.7740	0.7695	0.3474	1.0469	20, 20	15, 15	0.7746	0.7689	0.3532	1.0231	14, 14	11, 11	0.7088	0.7040	0.3088	1.1138
20, 21	15, 16	0.7737	0.7699	0.3434	1.0580	20, 21	15, 16	0.7739	0.7685	0.3437	1.0113	14, 15	11, 12	0.7085	0.7041	0.3069	1.1151
21, 20	16, 15	0.7729	0.7700	0.3308	1.0599	21, 20	16, 15	0.7765	0.7685	0.3621	1.0126	15, 14	12, 11	0.7080	0.7041	0.3013	1.1152
21, 21	16. 16	0.7737	0.7708	0.3440	1.0875	21, 21	16, 16	0.7734	0.7687	0.3389	1.0170	15, 15	12, 12	0.7084	0.7040	0.3054	1.1138
21, 22	16, 17	0.7737	0.7701	0.3434	1.0639	22, 21	16, 17	0.7726	0.7686	0.3245	1.0139	15, 16	12, 13	0.7081	0.7057	0.3022	1.1529
22, 21	17, 16	0.7735	0.7702	0.3407	1.0652	21, 22	17, 16	0.7741	0.7686	0.3477	1.0143	16, 15		0.7083		0.3045	
22, 22	17, 17	0.7740	0.7703	0.3473	1.0699	22, 22	17, 17	0.7685	0.7682	0.2237	1.0012	16, 16		0.7083		0.3046	
	17, 18		0.7700		1.0604		17, 18		0.7685		1.0132						

TABLE V. Padé approximant estimates of the critical temperatures u_c and the critical exponents γ' and β from $d/du \log M_0(u)$ and $d/du \log \chi_0(u)$ for the two-dimensional lattices with two equivalent neighbor interactions.

[M, N]		Δ(1, 2)				[M, N]		s.q.(1, 2)			
M_0	χ_0	u_c from M_0	u_c from χ_0	β	γ'	M_0	χ_0	u_c from M_0	u_c from χ_0	β	γ'
8, 8	5, 5	0.6465	0.6825	0.2234	1.5450	4, 4	3, 3	0.4670	0.4164	0.1377	0.7223
9, 9	6, 6	0.6556	0.7021	0.2634	1.7604	4, 5	3, 4	0.4730	0.4682	0.1488	1.3193
10, 10	7, 7	0.6522	0.6358	0.2455	1.0000	5, 4	4, 3	0.4772	0.4438	0.1583	0.9745
11, 11	7, 8	0.6807	0.6390	0.3057	1.0444	5, 5	4, 4	0.4801	0.4358	0.1659	0.8889
11, 12	8, 7	0.6462	0.6382	0.2127	1.0331	5, 6	4, 5	0.4759	0.4330	0.1545	0.8555
12, 11	8, 8	0.6531	0.6361	0.2521	1.0043	6, 5	5, 4	0.4778	0.4320	0.1597	0.8415
12, 12	8, 9	0.6368	0.6292	0.1527	0.9127	6, 6	5, 5	0.4740	0.4351	0.1498	0.8810
12, 13	9, 8	0.6825	0.6027	0.2770	0.5156	6, 7	5, 6	0.4801	...	0.1612	...
	9, 9	0.6120	0.6019	0.0406	0.5048	7, 6	6, 5	0.4661	0.4408	0.1242	0.9558
13, 12	9, 10	0.6247	0.6087	0.0847	0.6079	7, 7	6, 6	0.4699	0.4106	0.1378	0.8264
	10, 9	0.7078	0.6026	0.2886	0.5148	7, 8		0.4694		0.1360	
13, 13	10, 10	0.6249	0.6279	0.0856	0.9964	8, 7		0.4695		0.1363	
		0.7085		0.2893							

to be largely determined by the extent of the configurational information embedded in the expansion coefficients, and the n.n. model series for M_0 and χ_0 so far developed actually contain more information of this type.

As expected, the results for the three-dimensional lattices in Tables IV and VI are much smoother than those for the two-dimensional lattices; this is due to the larger number of terms available. The estimates for the critical point u_c obtained from M_0 and $\bar{\chi}_0$ appear to be converging to a common value for the three-dimensional lattices; the higher-order approximants of these functions yield agreement to two significant figures. Independent estimates of the critical point J/kT_c for the equivalent neighbor model lattices have been given by Domb and Dalton[14] who used the high-temperature ($T > T_c$) susceptibility series as a basis for extrapolation. Extrapolations from above T_c, where the ratio methods of Domb and Sykes[24] can be used, are generally more consistent in the estimates of the critical point than the corresponding extrapolations from below T_c. In Table VII we list the most likely values of $2J/kT_c$ and u_c to four significant figures.

The results for the critical exponents β and γ' of the two-dimensional lattices shown in Table V are too erratic to yield meaningful bounds; however, for the three-dimensional $L(1, 2)$ lattices, β appears to be settling down between 0.30 and 0.34, and γ' between 1.00 and 1.11. The estimates of γ' in Table IV are

TABLE VI. Padé approximant estimates of the critical temperatures u_c and the critical exponents γ' and β from $d/du(\log M_0)$ and $d/du(\log \chi_0)$ for the b.c.c.(1, 2, 3) and s.c.(1, 2, 3) lattices.

[M, N]		b.c.c.(1, 2, 3)				[M, N]		s.c.(1, 2, 3)			
M_0	χ_0	u_c from M_0	u_c from χ_0	β	γ'	M_0	χ_0	u_c from M_0	u_c from χ_0	β	γ'
24, 24	19, 19	0.8444	0.8580	0.3959	1.4653	24, 24	19, 19	0.8441	0.8578	0.3912	1.4602
24, 25	19, 20	0.8442	0.8610	0.3930	1.5447	24, 25	19, 20	0.8439	0.8610	0.3889	1.5446
25, 24	20, 19	0.8436	0.8579	0.3841	1.4622	25, 24	20, 19	0.8431	0.8579	0.3761	1.4631
25, 25	20, 20	0.8438	0.8619	0.3874	1.5605	25, 25	20, 20	0.8433	0.8619	0.3799	1.5603
25, 26	20, 21	0.8440	0.8473	0.3895	1.2184	25, 26	20, 21	0.8435	0.8459	0.3825	1.1875
26, 25	21, 20	...	0.8632	...	1.5785	26, 25	21, 20	...	0.8631	...	1.5782
28, 28	21, 21	0.8483	0.8476	0.4886	1.2257	28, 28	21, 21	0.8435	0.8461	0.3825	1.1944
28, 29	21, 22	0.8442	0.8474	0.3927	1.2198	28, 29	21, 22	0.8435	0.8459	0.3820	1.1886
29, 28	22, 21	...	0.8465	...	1.1916	29, 28	22, 21	0.8453	0.8448	0.4167	1.1541
29, 29	22, 22	0.8440	0.8479	0.3898	1.2364	29, 29	22, 22	0.8438	0.8466	0.3883	1.2090
29, 30	22, 23	0.8441	0.8471	0.3925	1.2108	29, 30	22, 23	0.8437	0.8456	0.3856	1.1783
30, 29	23, 22	0.8468	0.8341	0.4482	0.7532	30, 29	23, 22	0.8435	0.8343	0.3827	0.7976
30, 30	23, 23	0.8445	0.8401	0.3997	0.9726	30, 30	23, 23	0.8438	0.8379	0.3877	0.9248
30, 31	23, 24	0.8443	0.8396	0.3941	0.9538	30, 31	23, 24	0.8438	0.8383	0.3874	0.9372
31, 30	24, 23	0.8413	0.8397	0.3481	0.9563	31, 30	24, 23	0.8438	0.8383	0.3873	0.9392
	24, 24		0.8400		0.9675		24, 24		0.8377		0.9183

TABLE VII. Over-all best estimate of the critical points of the $L(1, 2)$ and $L(1, 2, 3)$ lattices.

Lattice	f.c.c.(1, 2)	b.c.c.(1, 2)	s.c.(1, 2)	$\Delta(1, 2)$	s.q.(1, 2)
u_c	0.7727	0.7092	0.7724	0.6349	0.4675
$2J/kT_c$	0.06445	0.08592	0.06450	0.1136	0.1901
Lattice	f.c.c.(1, 2, 3)	b.c.c.(1, 2, 3)	s.c.(1, 2, 3)	$\Delta(1, 2, 3)$	s.q.(1, 2, 3)
u_c	0.9023	0.8423	0.8413	0.7522	0.6351
$2J/kT_c$	0.0257	0.0429	0.0432	0.0712	0.1135

surprisingly consistent (more so than for the n.n. series) and also consistently lower than the value of $1\frac{5}{16}$ suggested by Baker and Gaunt. The above figures are only an initial approximation to the bounds on β and γ', and it is well known that the residues at the singularities of the approximants are extremely sensitive to the location of the pole. A variation of ϵ in u_c is usually amplified to 10ϵ in β and γ'. For the s.c.(1, 2, 3) and b.c.c.(1, 2, 3) lattices the estimates of γ' are less smooth but also consistently lower than $1\frac{5}{16}$; however, the values of β are higher than those of the $L(1, 2)$ lattices.

We can hope for a sequence of improved estimates of β and γ' if we have available independent estimates of u_c such as those in Table VII. The procedure is to evaluate the Padé approximants of

$$(u - u_c)\frac{d}{du}\log M_0(u) \sim \beta + (u - u_c)\frac{d}{du}\log D(u)\big|_{u\to u_c} \quad (38)$$

and

$$(u - u_c)\frac{d}{du}\log \chi_0(u) \sim -\gamma' + (u - u_c)\frac{d}{du}\log C(u)\big|_{u\to u_c} \quad (39)$$

at $u = u_c$. We have obtained values of β and γ' in this manner using the values of u_c in Table VII; the results for the two- and three-dimensional $L(1, 2)$ lattices are shown in Table VIII, and those for the s.c.(1, 2, 3) and b.c.c.(1, 2, 3) lattices in Table IX. We expect the critical points in Table VII to be correct to within at most 3 parts in 10^4, and the fluctuations in β and γ' resulting from this degree of uncertainty in u_c are approximately 4 parts in 10^3 throughout the Tables VIII and IX.

In the case of the s.q.(1, 2) lattice there are six low-temperature polynomials available and the estimates of β from the higher-order approximants suggest that the index is the same as the exact value of $\frac{1}{8}$ on the n.n. model two-dimensional lattices. For the $\Delta(1, 2)$ lattice, only five polynomials are available; consequently, we adopt the evidence from the s.q.(1, 2) lattice and conclude that

$$0.122 \leq \beta \leq 0.134 \quad (40)$$

for the two-dimensional $L(1, 2)$ lattices, and is probably exactly $= \frac{1}{8}$ as in the n.n. model. The estimates of γ' for the two-dimensional $L(1, 2)$ lattices have not improved; there is still too much scatter to make any conclusion. The figures in Table VIII for the three-dimensional lattices certainly suggest that the index β is not affected by extending the range of interactions. We conclude that

$$0.308 \leq \beta \leq 0.328, \quad (41)$$

which covers all the lattices and includes the effects of uncertainties in u_c. The bounds in (41) are wider than those of Baker and Gaunt,[35] but are similar to the earlier work of Essam and Fisher.[23] If indeed β is a rational fraction like $\frac{5}{16}$ as suggested by these authors, then it would appear safe to conclude that the same rational fraction is valid for the $L(1, 2)$ lattices.

The results for γ' of the b.c.c.(1, 2) lattices are very suggestive; the last four diagonal approximants yield $\gamma' = 1.212$, 1.211, 1.232, and 1.259, respectively. The estimates for the s.c.(1, 2) lattice are still erratic for the higher-order approximants; on the basis of the results for the b.c.c.(1, 2) and f.c.c.(1, 2) lattices, we conclude that

$$1.18 \leq \gamma' \leq 1.28. \quad (42)$$

In (42) it can be seen that we are slightly at odds with the estimate (35) of Baker and Gaunt[35] and the suggestion that $\gamma' = 1\frac{5}{16}$. The results for β in (41) and those of the high-temperature susceptibility index γ in Sec. VI strongly support the view that these exponents are not affected by including second neighbor interactions; consequently, we expect γ' to be similarly unaffected. The center of the range of uncertainty in (42) lies closer to the value $\gamma' = \frac{5}{4}$, and the value of $1\frac{5}{16}$ would appear to be excluded by our results, especially those for the b.c.c.(1, 2) lattice.

There is an important issue involved here, namely, the symmetry of the thermodynamic functions about

TABLE VIII. Estimates of the critical exponents β and γ' from the Padé approximants to Eqs. (38) and (39).

[M, N]		f.c.c.(1, 2)		[M, N]		s.c.(1, 2)		[M, N]		b.c.c.(1, 2)		[M, N]		Δ(1, 2)		[M, N]		s.q.(1, 2)	
M_0	χ_0	β	γ'	M_0	χ_0	β	γ'	M_0	χ_0	β	γ'	M_0	χ_0	β	γ'	M_0	χ_0	β	γ'
16, 16	11, 11	0.3315	0.7782	16, 16	11, 11	0.3269	0.7558	10, 10	6, 6	0.3120	0.8071	8, 8	5, 5	0.1815	0.3818	4, 4	2, 2	0.1387	1.2037
16, 17	11, 12	0.3252	...	16, 17	11, 12	0.3191	0.5761	10, 11	6, 7	0.3126	0.5454	8, 9	5, 6	0.1906	0.9426	4, 5	2, 3	0.1386	1.1525
17, 16	12, 11	...	...	17, 16	12, 11	0.3067	0.5783	11, 10	7, 6	0.3126	0.5482	9, 8	6, 5	0.1831	0.9606	5, 4	3, 2	0.1366	1.1582
17, 17	12, 12	0.3352	0.8562	17, 17	12, 12	0.3310	0.8175	11, 11	7, 7	0.3124	0.8000	9, 9	6, 6	0.2914	1.2727	5, 5	3, 3	0.1526	1.1889
17, 18	12, 13	0.3446	1.1342	17, 18	12, 13	0.3486	1.1219	11, 12	7, 8	0.3123	1.3287	9, 10	6, 7	0.1583	0.9899	5, 6	3, 4	0.1341	1.3078
18, 17	13, 12	0.3401	1.1376	18, 17	13, 12	0.3410	1.1254	12, 11	8, 7	0.3123	1.3412	10, 9	7, 6	0.1449	1.0032	6, 5	4, 3	0.1304	1.4927
18, 18	13, 13	0.3334	1.1267	18, 18	13, 13	0.3247	1.1129	12, 12	8, 8	0.3123	1.0225	10, 10	7, 7	0.1284	0.9885	6, 6	4, 4	0.1292	1.0820
18, 19	13, 14	0.3074	1.0896	18, 19	13, 14	0.3097	1.0600	12, 13	8, 9	0.3187	1.2115	10, 11	7, 8	0.1395	0.9903	6, 7	4, 5	0.1295	0.7208
19, 18	14, 13	0.3788	1.1119	19, 18	14, 13	0.3035	1.0930	13, 12	9, 8	0.3130	1.2162	11, 10	8, 7	0.1369	0.9797	7, 6	5, 4	0.1295	0.8721
19, 19	14, 14	0.3235	1.1228	19, 19	14, 14	0.3151	1.1080	13, 13	9, 9	0.3123	1.2116	11, 11	8, 8	0.1446	0.9873	7, 7	5, 5	0.1293	1.2376
19, 20	14, 15	0.3285	1.1272	19, 20	14, 15	0.3064	1.1131	13, 14	9, 10	0.3122	1.2115	11, 12	8, 9	0.1407	0.9892	7, 8	5, 6	0.1262	1.7492
20, 19	15, 14	0.3270	1.1288	20, 19	15, 14	0.2515	1.1146	14, 13	10, 9	0.3122	1.2077	12, 11	9, 8	0.1394	1.0001	8, 7	6, 5	0.1304	2.1042
20, 20	15, 15	0.3262	1.1344	20, 20	15, 15	0.3190	1.1206	14, 14	10, 10	0.3123	1.2112	12, 12	9, 9	0.1403	0.3658	8, 8	6, 6	0.1300	1.5035
20, 21	15, 16	0.3261	1.1615	20, 21	15, 16	0.3208	1.0709	14, 15	10, 11	0.3119	1.2114	12, 13	9, 10	0.1406	1.1622				
21, 20	16, 15	0.3260	0.7951	21, 20	16, 15	0.3207	1.1024	15, 14	11, 10	0.3118	1.2149	13, 12	10, 9	0.1386	1.1801				
21, 21	16, 16	0.3262	1.1701	21, 21	16, 16	0.3203	1.2125	15, 15	11, 11	0.3131	1.2321	13, 13	10, 10	0.5962	1.1785				
21, 22	16, 17	0.3246	1.1599	21, 22	16, 17	0.3202	0.9991	15, 16	11, 12	0.3089									
22, 21	17, 16	0.3388	1.2377	22, 21	17, 16	0.3201	1.0633	16, 15	12, 11	0.3071	1.1245								
22, 22	17, 17	0.3255	1.2230	22, 22	17, 17	0.3203	0.9557	16, 16	12, 12	0.3859	1.2587								
	17, 18		1.1777		17, 18		1.0021												
	18, 17		1.2391		18, 17		1.0839												

TABLE IX. Estimates of the critical exponents β and γ' from the Padé approximants to (38) and (39).

[M, N]		b.c.c.(1, 2, 3)		[M, N]		s.c.(1, 2, 3)	
M_0	χ_0	β	γ'	M_0	χ_0	β	γ'
25, 25	19, 19	0.3635	0.5814	25, 25	19, 19	0.3497	0.1963
25, 26	19, 20	0.3642	0.7622	25, 26	19, 20	0.3506	0.7247
26, 25	20, 19	0.3642	0.7622	26, 25	20, 19	0.3506	0.7248
26, 26	20, 20	0.3402	0.8114	26, 26	20, 20	0.2716	0.7764
26, 27	20, 21	0.2645	1.0614	26, 27	20, 21	0.1656	1.0494
27, 26	21, 20	0.2645	1.0633	27, 26	21, 20	0.1655	1.0515
27, 27	21, 21	0.3401	1.0530	27, 27	21, 21	0.2716	1.0421
27, 28	21, 22	0.3646	1.0280	27, 28	21, 22	0.3505	1.0262
28, 27	22, 21	0.3646	1.0370	28, 27	22, 21	0.3505	1.0315
28, 28	22, 22	0.3613	1.0478	28, 28	22, 22	0.3495	1.0388
28, 29	22, 23	0.3637	1.0521	28, 29	22, 23	0.3516	1.0426
29, 28	23, 22	0.3637	1.0531	29, 28	23, 22	0.3515	1.0437
29, 29	23, 23	0.3630	1.0558	29, 29	23, 23	0.3486	1.0507
29, 30	23, 24	0.3642	1.0394	29, 30	23, 24	0.3413	1.0838
30, 29	24, 23	0.3642	1.0494	30, 29	24, 23	0.3411	1.1441
30, 30	24, 24	0.3622	1.0655	30, 30	24, 24	0.3495	1.0598
30, 31		0.3625		30, 31		0.2636	
31, 30		0.3625		31, 30		0.2273	

the critical point. The scaling laws of Kadanoff[41] and Widom[42] predict equal values for the exponents above and below T_c, i.e., $\gamma = \gamma'$ and $\alpha = \alpha'$, etc. The value of γ is better established at 1.250 ± 0.003 than any other index both for our own equivalent neighbor model lattices and for the n.n. model. The symmetry of $\bar{\chi}_0$ about T_c is almost rigorously established for the two-dimensional nearest neighbor model lattices; consequently, for $\gamma' = 1\frac{5}{16}$ a breakdown of symmetry is indicated in three dimensions. We conclude that our own figures are inconsistent with this interpretation, that γ' is probably $\frac{5}{4}$, and that the transition is symmetric.

To further investigate the rival claims of $\gamma' = \frac{5}{4}$ or $\gamma' = 1\frac{5}{16}$, we can examine the approximants of $(\bar{\chi}_0)^{\frac{4}{5}}$ and $(\bar{\chi}_0)^{\frac{16}{21}}$. The function $(\bar{\chi}_0)^{1/\gamma'}$ has a simple pole at $u = u_c$, and following Baker[5] we expect greater consistency in the poles of the sequence of approximants if γ' is chosen correctly. The differences between the values of u_c obtained in this way and the values shown in Table VII are listed in Table X (the differences are recorded in units of 10^{-4}). We have taken the sequence of $[N, N+1]$ approximants in each case. The two sequences in Table X indicate that the assumption $\gamma' = \frac{5}{4}$ is more consistent with the high-temperature estimates of u_c.

The evidence from Tables VI and IX indicates that β is significantly higher for the third equivalent neighbor model lattices and suggests that

$$0.345 \leq \beta \leq 0.365 \tag{43}$$

for the s.c.(1, 2, 3) and b.c.c.(1, 2, 3) lattices. The corresponding values of γ' suggested by Table IX are

$$1.01 \leq \gamma' \leq 1.14. \tag{44}$$

In the light of the results for the $L(1, 2)$ lattices, the estimates of β for the s.c.(1, 2, 3) and b.c.c.(1, 2, 3) lattices are puzzling, also the values of γ' are significantly lower than expected. We cannot say that (43) and (44) represent a definite extended-range effect, only that the bounds have been established in exactly the same manner as those above and those of previous authors. Two points must be made here. First, these estimates are based on expansions involving low-temperature spin configurations containing a maximum of five spins. In the corresponding series for the $L(1, 2)$ lattices several configurations of six and seven spins were included (see above) by extending the series. Second, if the partition function is nonuniformly convergent in the range of interaction, progressively more terms in the expansions are required to obtain a given accuracy in the estimates of critical parameters such as γ' and β. The authors are therefore inclined to the view that the indices are unchanged by the inclusion of higher neighbor interactions.

If the shift between the ranges (41) and (43), and (42) and (44) is not all accounted for by the above convergence effect, then (43) may have some bearing on the gas–liquid critical point. It has often been suggested that discrepancies between values of β obtained from coexistence curve measurements and the values based on the n.n. Ising model are due to the site restrictions of atoms in the Ising model. One way of examining this is to adopt the quantum-lattice gas model of Matsubara and Matsuda,[43] taking into account the kinetic energy of the gas molecules. The magnetic analog of the quantum-lattice gas is the anisotropic Heisenberg model. Preliminary work on this model by the present authors[44] and Fisher[45] indicates that for the molecules found in nature a removal of the site restriction is likely to have no effect on the critical exponents. The value of β obtained by Fisher[46] in an analysis of Weinberger and Schneider's[47] data on xenon is $\beta = 0.345 \pm 0.015$, which falls in the range (43). It seems very likely that the quantum-lattice gas will not account for these discrepancies, and in view of (43) an Ising-lattice gas model with hard cores of a larger size

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[47] M. A. Weinberger and W. G. Schneider, Can. J. Chem. **30**, 422 (1952).

TABLE X. Difference between u_c obtained from the $[N, N+1]$ approximants to $(\chi_0)^{1/\gamma'}$ and the values in Table VII.

N	f.c.c.(1, 2)		N	s.c.(1, 2)		N	b.c.c.(1, 2)	
	$\gamma' = \frac{5}{4}$	$\gamma' = 1\frac{5}{16}$		$\gamma' = \frac{5}{4}$	$\gamma' = 1\frac{5}{16}$		$\gamma' = \frac{5}{4}$	$\gamma' = 1\frac{5}{16}$
11	163	200	11	265	...	6	41	79
12	69	100	12	75	105	7	98	138
13	50	75	13	56	80	8	58	96
14	51	76	14	56	80	9	17	42
15	26	47	15	11	43	10	18	43
16			16	150	−72	11	1	23
17	24	−29	17	3	−76	12	−44	−22

together with an attractive potential of an extended range may be the answer, where, for example, the core prevents simultaneous occupation of first neighbor sites and attractive interactions are present up to third neighbors.

V. HIGH-TEMPERATURE SERIES EXPANSIONS

An extensive literature exists on the high-temperature development of the Ising model; a complete set of references can be found in reviews by Domb[2] and Fisher.[5] The calculations proceed by expanding the partition function in the form

$$Z_N = \mathrm{Tr}\, e^{-\beta\mathcal{H}} = \sum_n \mathrm{Tr}\,\{\mathcal{H}^n\}(-1)^n\beta^n/n! \quad (45)$$

and isolating the contributions to successive terms in the form of high-temperature lattice constants. Recent calculations of Sykes, Essam, Heap, and Hiley[48] have considerably extended the number of high-temperature lattice constants available for the nearest neighbor model, and Sykes, Martin, and Hunter[49] have employed these to extend the specific-heat C_v expansion for the f.c.c.(1) lattice. These authors find that C_v diverge at the critical point as

$$C_v \sim B(T - T_c)^{-\alpha}, \quad (46)$$

where α (the high-temperature specific-heat exponent) $\simeq \frac{1}{8}$.

The high-temperature expansions for the second and third equivalent neighbor model lattices have been derived by Domb and Dalton,[14] who obtained the high-temperature expansions of the zero-field partition function and susceptibility for the second equivalent neighbor model to order T^{-7} and similarly for the third equivalent neighbor model to order T^{-6}. These authors discussed the "bulk" critical properties such as the critical energy and entropy, and examined their asymptotic behavior for large coordination numbers. Finally, Dalton[15] derived the expansions of the zero-field partition function and susceptibility, valid for general spin and arbitrary second neighbor exchange interaction through to orders T^{-6} and T^{-5}, respectively.

It is our purpose to examine the dependence of the bulk critical properties of the second neighbor model ($S = \frac{1}{2}$) upon the relative strengths of the nearest neighbor and next nearest neighbor interactions; for this we introduce the parameter $\alpha = J_2/J_1$. We also examine the high-temperature susceptibility critical exponent γ for the equivalent neighbor model lattices.

The high-temperature expansions of the zero-field susceptibility and partition function for the second neighbor model are in the form

$$kT\chi_0/Nm^2 = 1 + \sum_{n=0}^{\infty} c_n(\alpha)K^n \quad (47)$$

and

$$\ln Z/N = \ln 2 + \sum_{n=0}^{\infty} b_n(\alpha)K^n, \quad (48)$$

where $K = 2J_1/kT$ and the coefficients $c_n(\alpha)$ and $b_n(\alpha)$ are polynomials of degree n in α. The expansions can be conveniently reduced to a general form valid for an arbitrary regular lattice, where they are expressed in terms of q_1, q_2 and the lattice constants of multiply connected diagrams. These expansions are recorded in Appendix D.

VI. VARIATION OF THE CRITICAL TEMPERATURE WITH THE SECOND NEIGHBOR INTERACTION

For the second neighbor model we have investigated the variation of $K_c\,(= J_1/kT_c)$ with $\alpha\,(= J_2/J_1)$ for values of α in the range $0 \leq \alpha \leq 1$ (both J_1 and J_2 positive). To determine the critical temperatures, the Padé approximants to $d/dK \ln(\bar{\chi}_0)$ and $(\bar{\chi}_0)^{\frac{4}{5}}$ have been calculated and the appropriate singularities selected. The higher-order approximants to both these

[48] M. F. Sykes, J. W. Essam, B. R. Heap, and B. J. Hiley, J. Math. Phys. **7**, 1557 (1966).
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TABLE XI. Values of $2J_1/kT_c(\alpha)$ based on the [3, 3] approximants to $(\chi_0)^{\frac{4}{5}}$ for the three-dimensional lattices and $(\chi_0)^{\frac{4}{7}}$ for the two-dimensional lattices.

α	f.c.c.	s.c.	b.c.c.	Δ	s.q.
0	0.1021	0.2216	0.1573	0.2743	0.4418
0.1	0.09624	0.1759	0.1450	0.2375	0.3870
0.2	0.09123	0.1465	0.1344	0.2132	0.3451
0.3	0.08638	0.1258	0.1253	0.1906	0.3118
0.4	0.08231	0.1107	0.1175	0.1729	0.2849
0.5	0.07862	0.09645	0.1106	0.1587	0.2625
0.6	0.07527	0.08904	0.1045	0.1468	0.2436
0.7	0.07223	0.08123	0.09914	0.1368	0.2274
0.8	0.06944	0.07474	0.09430	0.1282	0.2134
0.9	0.06689	0.06925	0.08994	0.1207	0.2010
1.0	0.06453	0.06452	0.08599	0.1140	0.1902

functions yield agreement in K_c to within 3 parts in 10^4 over the whole range of α for the lattices in Table XI. The agreement always improves with increasing values of α and is as little as 1 part in 10^4 for the three-dimensional lattices with $\alpha > \frac{1}{4}$. In Table XI we present the estimates of $K_c(\alpha)$ based on the [3, 3] approximants to $(\chi_0)^{\frac{4}{5}}$ for the three-dimensional lattices, and to $(\chi_0)^{\frac{4}{7}}$ for the two-dimensional lattices.

The variation of the critical temperature with the strength of the second neighbor interaction is shown in Figs. 3 and 4 where $T_c(\alpha)/T_c(0)$ is plotted against

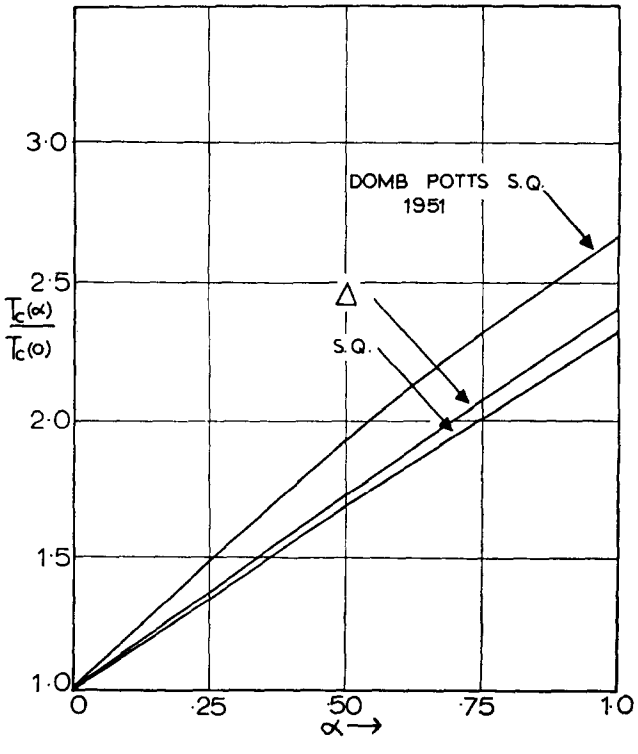

FIG. 3. The variation of the critical point for the s.q. and triangular lattices for values of α in the range $0 \leq \alpha \leq 1$.

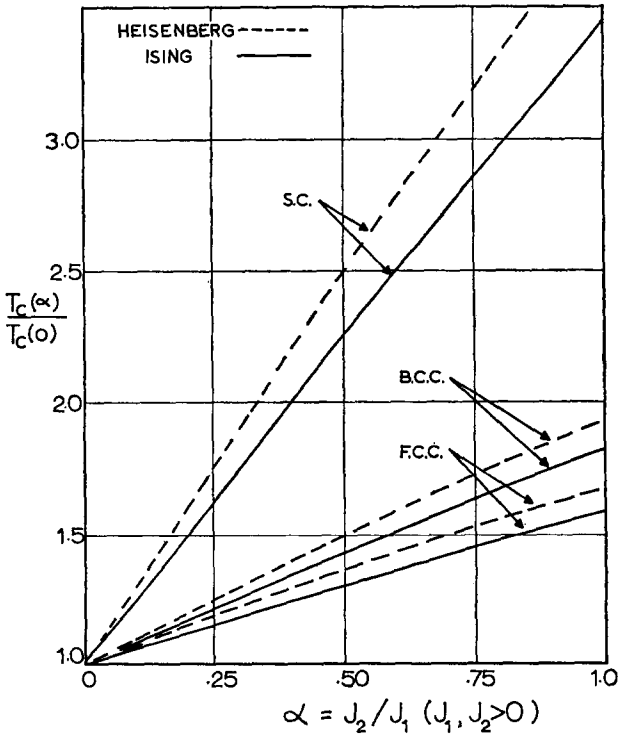

FIG. 4. The variation of the critical point of the three-dimensional lattices for the Heisenberg and Ising models with α in the range $0 \leq \alpha \leq 1$. The curves for the Heisenberg model are taken from Dalton and Wood.[23]

α for the two- and three-dimensional lattices, respectively. Here $T_c(0)$ is the critical temperature of the n.n. model. In Fig. 3 the results of Domb and Potts[13] for the s.q. lattice are shown for comparison, and in Fig. 4 we compare the corresponding curves for the Heisenberg model obtained by the present authors.[23] The plots do show a slight curvature which is more pronounced for the two-dimensional lattices and is very likely due to the more rapid convergence for $\alpha \geq \frac{1}{4}$. To a good approximation, the variation of the critical temperature in the range $0 \leq \alpha \leq 1$ can be represented by

$$T_c(\alpha) = T_c(0)\{1 + m_1\alpha\}, \tag{49}$$

where the values of m_1 obtained from Figs. 3 and 4 are compared with the corresponding values for the Heisenberg model ($S = \frac{1}{2}$) in Table XII. The values of m_1 given here for the Ising model reproduce the

TABLE XII. Estimates of m_1 in (49) for the Heisenberg and Ising models.

Lattice	f.c.c.	s.c.	b.c.c.	s.q.	Δ'
Ising	0.61	2.47	0.84	1.45	1.35
Heisenberg	0.69	2.80	0.94	—	—
Classical	0.50	2.00	0.75	2.00	2.00

critical temperatures to within 2% for the two-dimensional lattices and to within 1% for the three-dimensional lattice. The classical theories of both the Ising and Heisenberg models predict that $T_c(\alpha)/T_c(0)$ is exactly linear in α with m_1 given by

$$m_1 = q_2/q_1. \tag{50}$$

Interesting effects occur when $\alpha < 0$ with $J_1 > 0$ and $J_2 < 0$, and the question of the type of antiferromagnetic ordered state arises. In the case of the Heisenberg model this problem has recently been considered by Tahir-Kheli, Callen, and Jarrett[50] using a first-order Green-function treatment, the results of which agree well with a series-expansion approach discussed by the present authors.[51] The results indicate that $T_c(\alpha) \to 0$ as $\alpha \to \alpha^*$, where for $\alpha < \alpha^*$ ferromagnetic ordering gives way to some kind of antiferromagnetic ordering. Unfortunately, the present expansions ($S = \frac{1}{2}$) of the susceptibility quickly become erratic for α in the range $-1 \leq \alpha \leq 0$, and we can only suggest the following limits on α^*;

$$\text{f.c.c.} \quad -1.0 \leq \alpha^* \leq -0.7, \tag{51a}$$

$$\text{s.c.} \quad -0.4 \leq \alpha^* \leq -0.2, \tag{51b}$$

$$\text{b.c.c.} \quad -0.8 \leq \alpha^* \leq -0.6. \tag{51c}$$

It is highly probable that α^* is independent of spin and that by examining the general spin expansions given by Dalton, α^* could be obtained to within a few per cent.

VII. THE CRITICAL EXPONENT OF THE HIGH-TEMPERATURE SUSCEPTIBILITY

The high-temperature approach to T_c of $\bar{\chi}_0$ is of the form

$$\chi_0 \sim E(T - T_c)^{-\gamma}\big|_{T \to T_c^+}, \tag{52}$$

where γ is the critical exponent and E the amplitude of the singularity. Of all the critical exponents related to the three-dimensional n.n. model lattices this is the most firmly established on the basis of series expansions. The conclusion of the numerical work is

$$\gamma = 1.250 \pm 0.003 \simeq 1\tfrac{1}{4}, \tag{53}$$

and it is suggested that $\gamma = 1\frac{1}{4}$ exactly. For the two-dimensional lattices, $\gamma = 1\frac{3}{4}$. (See Ref. 52.)

The expansions of χ_0 above T_c are very suitable for extrapolation, since the terms of the expansion are all positive and display a smooth behavior. Consequently, we can employ the ratio methods of Domb and Sykes[24] to obtain estimates of γ for the $L(1, 2)$ and $L(1, 2, 3)$ lattices. The values of K_c for these lattices have been given previously by Domb and Dalton.[14] Following Domb and Sykes[24] the coefficients c_n in (47) are assumed to have the asymptotic form

$$c_n \sim Cn^{\gamma-1}K_c^{-n}, \tag{54}$$

where C is some constant. From (54) we can form the sequence $\{\gamma_n\}$, where

$$\gamma_n = 1 + nK_c(\mu_n - 1/K_c) \tag{55}$$

and

$$\mu_n = c_n/c_{n-1},$$

yielding successive estimates of γ. The values of K_c in (55) should be the over-all best estimates given in Table VII. In Table XIII and XIV we record these results for γ for the $L(1, 2)$ and $L(1, 2, 3)$ lattices, respectively. The sequences $\{\gamma_n\}$ appear to be increasing to limiting values for both the $L(1, 2)$ and $L(1, 2, 3)$ lattices. The figures for the s.q.(1, 2) lattice certainly suggest that $\gamma = 1\frac{3}{4}$, the same value as for the n.n. model lattices. Again, assuming γ to be a simple rational fraction, $\{\gamma_n\}$ for the three-dimensional $L(1, 2)$ lattices appear to be approaching a value of $\gamma = 1\frac{1}{4}$.

The sequences $\{\gamma_n\}$ for the $L(1, 2, 3)$ lattices are consistently lower than the corresponding sequences for the $L(1, 2)$ lattices, although they are converging at approximately the same rates. The figures for the s.c.(1, 2, 3) lattices suggest that the final limit is again likely to be $1\frac{1}{4}$.

We have also obtained estimates of γ by computing the Padé approximants to $d/dK[\log(\bar{\chi}_0)]$ and finding

TABLE XIII. Estimates of γ obtained from (55) for the second equivalent neighbor model lattices.

n	s.q.(1, 2) γ_n	Δ(1, 2) γ_n	s.c.(1, 2) γ_n	b.c.c.(1, 2) γ_n	f.c.c.(1, 2) γ_n
2	1.634	1.499	1.193	1.228	1.191
3	1.709	1.583	1.210	1.240	1.207
4	1.728	1.634	1.219	1.241	1.215
5	1.742	1.643	1.224	1.242	1.221
6	1.749	1.682	1.228	1.242	1.224
7	1.754	1.693	1.231	1.243	1.227
8	1.756				

TABLE XIV. Estimates of γ obtained from (55) for the third equivalent neighbor model lattices.

n	s.q.(1, 2, 3) γ_n	Δ(1, 2, 3) γ_n	s.c.(1, 2, 3) γ_n	b.c.c.(1, 2, 3) γ_n	f.c.c.(1, 2, 3) γ_n
2	1.497	1.421	1.160	1.145	1.107
3	1.580	1.514	1.186	1.163	1.127
4	1.630	1.574	1.199	1.176	1.140
5	1.662	1.614	1.210	1.184	1.150
6	1.681	1.642	1.219	1.190	1.167

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[51] D. W. Wood and N. W. Dalton, Phys. Rev. **159**, 384 (1967).
[52] L. P. Kadanoff, Nuovo Cimento **44**, 279 (1966).

TABLE XV. Estimates of the high-temperature susceptibility critical exponent γ obtained from the approximants to $d/dK\{\log \chi_0\}$ for the $L(1, 2)$ lattices.

[N, M]	s.q.(1, 2)	[N, M]	Δ(1, 2)	[N, M]	s.c.(1, 2)	[N, M]	b.c.c.(1, 2)	[N, M]	f.c.c.(1, 2)
2, 2	1.811	2, 2	2.559	2, 2	1.216	2, 2	1.248	2, 2	1.210
2, 3	1.825	2, 3	1.963	2, 3	1.221	2, 3	1.244	2, 3	1.226
3, 2	1.852	3, 2	1.441	3, 2	1.220	3, 2	1.245	3, 2	1.218
3, 3	1.836	3, 3	1.952	3, 3	1.227	3, 3	1.244	3, 3	1.221
4, 3	1.823	4, 2	1.955	4, 2	1.228	4, 2	1.244	4, 2	1.221
3, 4	1.832	2, 4	1.952	2, 4	1.224	2, 4	1.244	2, 4	1.221

TABLE XVI. Estimates of the high-temperature susceptibility critical exponent γ from the approximants to $d/dK\{\log \chi_0(K)\}$ for the $L(1, 2, 3)$ lattices.

[N, M]	s.q.-(1, 2, 3)	[N, M]	Δ-(1, 2, 3)	[N, M]	s.c.-(1, 2, 3)	[N, M]	b.c.c.-(1, 2, 3)	[N, M]	f.c.c.-(1, 2, 3)
2, 2	2.411	2, 2	2.166	2, 2	1.168	2, 2	1.181	2, 2	1.135
2, 3	2.411	2, 3	1.979	2, 3	1.262	2, 3	1.185	2, 3	1.144
3, 2	2.165	3, 2	1.949	3, 2	1.187	3, 2	1.184	3, 2	1.142

the residues at the appropriate singularities (see Sec. III). These results are shown in Tables XV and XVI. These sequences are less regular than those obtained using the ratio method; however, the results for the three-dimensional lattice are in excellent agreement with those of Tables XIII and XIV. From the results over-all, we conclude that the index γ is not affected by extending the range of interaction for either the two-dimensional or three-dimensional lattices. On the basis of the figures for the s.q.(1, 2) and b.c.c.(1, 2) lattices, we conclude that

$$\gamma = 1.25 \pm 0.01 \quad \text{(three dimensions)} \tag{56}$$

and

$$\gamma = 1.79 \pm 0.04 \quad \text{(two dimensions)}. \tag{57}$$

VIII. THE CRITICAL ENERGY AND ENTROPY

Those critical properties which change noticeably, with the type of exchange interactions present, the range of the interactions and their relative strengths, are of interest in relation to experimental work. From these properties information relating to specific materials can be deduced. The critical properties in this category are principally the critical point K_c; the critical energy $(E_\infty - E_c)/kT_c$, and the critical entropy $(S_\infty - S_c)/k$. The critical energy and entropy are particularly useful for comparing model calculations since they are independent of the exchange constant J_1, and in the case of the second neighbor model depend only on the relative magnitude of J_1 and J_2, and consequently can be used to detect the presence of n.n.n. interactions. Both functions are related to the area under the high-temperature specific-heat curves ("the tail") plotted on a reduced scale of temperature $t\,(= T/T_c)$; the relations are

$$(E_\infty - E_c)/kT_c = 1/k\int_1^\infty C_v\, dt \tag{58}$$

and

$$(S_\infty - S_c)/k = 1/k\int_1^\infty \frac{C_v}{t}\, dt. \tag{59}$$

Domb and Sykes[53] have examined the effects of spin on these functions for the Ising and Heisenberg n.n. model lattices and the present authors[23,44] have previously discussed the effects of n.n.n. interactions, and of anisotropic n.n. interactions for the three-dimensional Heisenberg lattices. We have also given a detailed comparison of the statistical theories with the experimental work of Miedema *et al.*[54] on the ferromagnetic salts $CuK_2Cl_42H_2O$ and $Cu(NH_4)_2Cl_42H_2O$, where by the use of (58) and (59) the exchange integrals J_1/k and J_2/k are estimated.[55] A review of such comparisons has been given by Domb and Miedema.[8]

The expansions of the critical energy and entropy can be obtained from the coefficients $P_{r,s}$ in Appendix D. For example, the expansions for the f.c.c. lattice are

$$\begin{aligned}\frac{E_\infty - E_c(\alpha)}{kT_c} = {} & (6 + 3\alpha^2)K_c^2 + (24 + 36\alpha)K_c^3 \\ & + (130 + 288\alpha + 144\alpha^2 + 11\alpha^4)K_c^4 \\ & + (800 + 2240\alpha + 2160\alpha^2 + 760\alpha^3)K_c^5 \\ & + (5316.8 + 18432\alpha + 24480\alpha^2 \\ & + 14400\alpha^3 + 3636\alpha^4 + 108.4\alpha^6)K_c^6,\end{aligned} \tag{60}$$

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TABLE XVII. Normalized estimates for $\frac{E_\infty - E_c(\alpha)}{kT_c}$: Ising model $s = \frac{1}{2}$.

α	f.c.c.(1, 2)	s.c.(1, 2)	b.c.c.(1, 2)	Δ(1, 2)	s.q.(1, 2)
0	0.150	0.237	0.169	0.549	0.623
0.1	0.140	0.181	0.159	0.482	0.580
0.2	0.134	0.158	0.150	0.470	0.545
0.3	0.125	0.137	0.143	0.435	0.519
0.4	0.119	0.129	0.137	0.409	0.503
0.5	0.111	0.123	0.135	0.387	0.491
0.6	0.109	0.122	0.134	0.370	0.482
0.7	0.105	0.117	0.132	0.358	0.473
0.8	0.101	0.109	0.131	0.346	0.465
0.9	0.099	0.103	0.130	0.337	0.460
1.0	0.098	0.098	0.129	0.330	0.456

TABLE XVIII. Normalized estimates for $\frac{S_\infty - S_c(\alpha)}{k}$: Ising model $s = \frac{1}{2}$.

α	f.c.c.(1, 2)	s.c.(1, 2)	b.c.c.(1, 2)	Δ(1, 2)	s.q.(1, 2)
0	0.102	0.152	0.107	0.363	0.387
0.1	0.096	0.130	0.104	0.342	0.377
0.2	0.090	0.104	0.100	0.325	0.366
0.3	0.085	0.102	0.096	0.314	0.358
0.4	0.081	0.094	0.094	0.296	0.352
0.5	0.078	0.086	0.093	0.285	0.349
0.6	0.075	0.081	0.092	0.279	0.344
0.7	0.072	0.076	0.090	0.275	0.339
0.8	0.069	0.072	0.089	0.270	0.336
0.9	0.067	0.069	0.087	0.261	0.334
1.0	0.065	0.065	0.086	0.250	0.332

and

$$\frac{S_\infty - S_c(\alpha)}{k} = (3 + 1.5\alpha^2)K_c^2 + (16 + 24\alpha)K_c^2 + (97.5 + 216\alpha + 108\alpha^2 + 8.25\alpha^4)K_c^4 + (640 + 1792\alpha + 1728\alpha^2 + 608\alpha^3)K_c^5 + (4430\tfrac{2}{3} + 15360\alpha + 20400\alpha^2 + 12000\alpha^3 + 3030\alpha^4 + 90\tfrac{1}{3}\alpha^6)K_c^6. \quad (61)$$

By forming the Padé approximants to these series and evaluating them at $K = K_c$ [values of $K_c(\alpha)$ are obtained from Table XI] we have obtained estimates of the critical energy and entropy in the range $0 \leq \alpha \leq 1$. These show a greater spread between successive approximants than the other parameters discussed above, the reason being that the series are quite short and the terms have not settled down to any smooth behavior. The longer series available for the points $\alpha = 0$ (n.n. model) and $\alpha = 1$ (second equivalent neighbor model) makes it possible to determine these critical parameters at each end of the range more accurately; and in the case of the two-dimensional lattices we have, of course, exact results at $\alpha = 0$. We can take advantage of this by fitting the critical-energy and entropy curves to pass through the end points using a normalization method described by us previously.[55] The normalized estimates are given in Tables XVII and XVIII. In Figs. 5 and 6 the

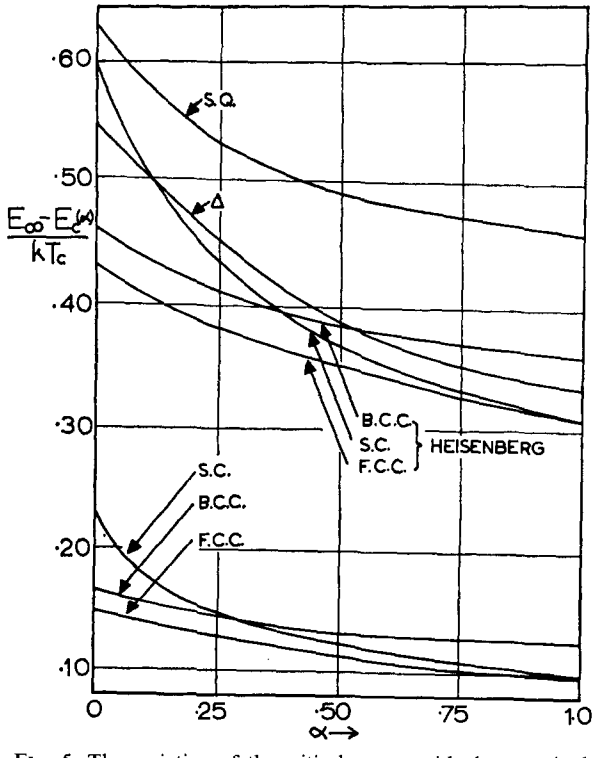


FIG. 5. The variation of the critical energy with the magnitude of the second neighbor interactions. The curves for the Heisenberg model are taken from Dalton and Wood.[23]

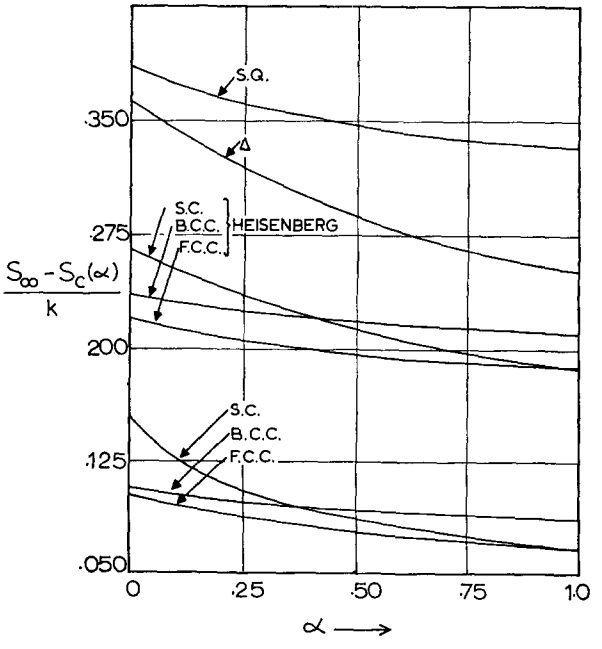


FIG. 6. The variation of the critical entropy with the magnitude of the second neighbor interactions. The curves for the Heisenberg model are taken from Dalton and Wood.[23]

critical-energy and entropy curves for the two- and three-dimensional lattices are shown, and compared with the corresponding curves for the Heisenberg model. The curves illustrate the rapid decrease of the specific-heat tail for the two-dimensional lattices on the inclusion of second neighbor interactions, and also the large differences in the tail on passing from two to three dimensions. The curves for the Heisenberg model in Figs. 5 and 6 illustrate the much larger tails on the C_v curves compared with the corresponding Ising model lattices.

IX. CONCLUSIONS

In this paper we have discussed some of the effects of more-distant-neighbor interactions on the critical and thermodynamic properties of the Ising ferromagnet. In considering the critical-point behavior of the model, we have made use of the concept of the equivalent neighbor model introduced by Domb and Dalton.[14] In this model the range of interaction is extended to include 2nd, 3rd, $\cdots$, nth neighbor interactions but the exchange constant is maintained at the same value between all the interactions taken into account. The equivalent neighbor model has been used to examine the critical exponents related to the magnetization M_0, and the low- and high-temperature ($T \gtrless T_c$) zero-field susceptibility χ_0 for the Ising model with second and third equivalent neighbor interactions present. Our philosophy has been that any detectable effects of an extended range of interaction on the critical exponents must be visible in the equivalent neighbor model, and that for this purpose it is unnecessary to consider finer details such as the relative strength of the interactions. The theoretical approach used is the one of developing power-series expansions for the partition function and related thermodynamic functions valid in regions above and below the transition temperature.

In Sec. II the development of the low-temperature expansion of the partition function Z_N with interactions between nth neighbor pairs present is described and specific consideration is given to the second neighbor model, where the high-temperature–low-temperature transformation of Domb[27] is applied to deriving the low-temperature polynomials $f_n(u, v)$ appearing in Z_N. The first five low-temperature polynomials are obtained for the second neighbor model two- and three-dimensional lattices (six polynomials in the particular case of the s.q. lattice). The same number of polynomials have also been determined for the second and third equivalent neighbor model lattice [except for the f.c.c.(1, 2, 3) where only four polynomials are available]. Some of the aspects related to the enumeration and counting of the low-temperature spin configurations contributing to the polynomials $f_n(u, v)$ are briefly discussed in Sec. III. The numerical data related to Secs. II and III is collected together in Appendices A, B, and C. These Appendices contain all the high-temperature polynomials $\varphi_{p,q}(\mu)$ [Eq. (15)] and low-temperature polynomials $g_n(u, v)$ [Eq. (13)] which have been derived; and also the low-temperature lattice constants of all the spin configurations (which can occur on the lattices considered) of up to five spins for the equivalent neighbor model lattices.

The critical exponents β and γ' relating to M_0 and χ_0 ($T < T_c$), respectively, are discussed in Sec. IV where the Padé-approximant techniques of Baker,[5] and Essam and Fisher[33] have been employed to form estimates for the equivalent neighbor model lattices. In the case of the two- and three-dimensional $L(1, 2)$ lattices, the estimates of β strongly support the view that this index remains unchanged from its value in the n.n. model lattices. The range of uncertainty in the over-all estimates (41) is such that no shift in β is detectable, and if β is a rational fraction then it is very likely to be the same rational fraction for the $L(1)$ and $L(1, 2)$ lattices. For the three-dimensional $L(1, 2)$ lattices we conclude that γ' lies within the limits (42) which excludes the value of $1\frac{5}{16}$ suggested by Baker and Gaunt[35] for the n.n. model lattices. For the b.c.c.(1, 2) lattice, the [13, 13], [14, 14], [15, 15], and [16, 16] approximants in Table VIII yield the estimates $\gamma = 1.212$, 1.211, 1.232, and 1.259, respectively. On the basis of these estimates and those of the other lattices, we conclude that γ' is probably $\frac{5}{4}$ if a rational fraction is sought, and that $\gamma' = \gamma$ for these lattices, thus supporting the view that χ_0 is symmetric through the transition in a similar manner to the two-dimensional n.n. lattices. We have pointed out the surprising values of β obtained in Table IX for the three-dimensional $L(1, 2, 3)$ lattices. These estimates have been obtained in exactly the same way as the other values of β and are summarized by (43), which covers the same width of uncertainty as (41) but which lies considerably above the value of $\frac{5}{16}$. On the basis of the numerical work alone, (43) should be regarded with "almost" the same degree of conviction as (41), but because of the nonuniform convergence of the series with respect to the range of interaction, these results are not as reliable as the corresponding results for the $L(1, 2)$ lattices, which support the authors' view that all the critical indices are independent of the range of force. If, however, the shift between the ranges (41) and (43) is not entirely a convergence effect and is in part a real effect,

then the results (43) and (44) may be able to explain some of the hitherto unexplained discrepancies between the experimental evidence for β and the theoretical predictions of the n.n. Ising model, which are of the same order as suggested by (43).

Sections V, VI, VII, and VIII are devoted to the high-temperature series expansions of the second neighbor model and equivalent neighbor models, and are concerned with the critical properties that can be deduced from them. The coefficients of Z_N and $\chi_0\,(T > T_c)$ for the second neighbor model are recorded in a generalized form in Appendix D, where the expansions are given through to terms in T^{-7} and T^{-6}, respectively ($S = \frac{1}{2}$). In Sec. VI the variation of the critical point with the parameter $\alpha\ (= J_2/J_1)$ is presented in the range $0 \leq \alpha \leq 1$. The results are compared with the corresponding behavior of the Heisenberg model, and like the Heisenberg model the variation of T_c is given to a good approximation by the linear relation

$$T_c(\alpha) = T_c(0)\{1 + m_1\alpha\} \quad (0 \leq \alpha \leq 1). \qquad (62)$$

These results are displayed in Figs. 3 and 4.

The high-temperature susceptibility exponent γ for the $L(1, 2)$ and $L(1, 2, 3)$ lattices is discussed in Sec. VII. Here both the ratio methods of Domb and Sykes[24] and the Padé-approximant methods are used. The ratio method yields smooth and increasing sequences $\{\gamma_n\}$ for estimates of γ. The results over-all and in particular $\{\gamma_n\}$ for the s.q.(1, 2) and b.c.c.(1, 2) lattices support the view that the index γ is unaffected by extending the range of interaction and that if γ is a rational fraction then it is the same rational fraction for the $L(1)$, $L(1, 2)$, and $L(1, 2, 3)$ lattice in both two and three dimensions.

Finally, in Sec. VIII we have presented estimates of the critical energy $(E_\infty - E_c)/kT_c$ and the critical entropy $(S_\infty - S_c)/k$ in the range $0 \leq \alpha \leq 1$ for the second neighbor model. We have included these functions along with $K_c(\alpha)$ because they are very useful in comparison with experimental work, where specific estimates of J_1/k and J_2/k are attempted on the basis of measurements of the magnetic specific heat above T_c. The figures in Tables XI, XVII, and XVIII can be used as a reliable basis for such comparisons. The variation of the critical energy and entropy is shown in Figs. 5 and 6 where the Ising model curves are compared with the corresponding Heisenberg model results. The authors have previously considered the effects anisotropy on $K_c(\alpha)$, $(E_\infty - E_c)/kT_c$ and $(S_\infty - S_c)/k$; and also their behavior for the second neighbor Heisenberg model. With this broad basis of numerical work it is hoped in a future publication to present a comprehensive examination of the recent experimental work on ferromagnetic insulators.

ACKNOWLEDGMENTS

We are very grateful to Professor C. Domb and to Dr. M. F. Sykes for the constant interest and advice they have given in this work. We would also like to express our thanks to the Universities of London and Nottingham Computer Units, and also to the Chilton Atlas Computer Laboratory.

APPENDIX A

Listed below are the high-temperature polynomials $\varphi_{r,q}(\mu)$ and the low-temperature polynomials $g_s(u, v)$ for the second neighbor model lattices. The polynomials are defined in Sec. II [Eqs. (13) and (14)] in relation to the low-temperature expansion of the partition function.

High-temperature polynomials for the s.c. lattice:

$$\varphi_{0,0} = 1,$$
$$\varphi_{1,0} = -3\mu,$$
$$\varphi_{0,1} = -6\mu,$$
$$\varphi_{2,0} = 3\mu - 6\mu^2 + 3\mu^3,$$
$$\varphi_{1,1} = 18\mu - 18\mu^2 + 18\mu^3,$$
$$\varphi_{0,2} = 15\mu - 21\mu^2 + 15\mu^3,$$
$$\varphi_{3,0} = -\mu + 25\mu^2 - 49\mu^3 + 25\mu^4 - \mu^5,$$
$$\varphi_{2,1} = -18\mu + 180\mu^2 - 312\mu^3 + 180\mu^4 - 18\mu^5,$$
$$\varphi_{1,2} = -45\mu + 369\mu^2 - 675\mu^3 + 369\mu^4 - 45\mu^5,$$
$$\varphi_{0,3} = -20\mu + 230\mu^2 - 414\mu^3 + 230\mu^4 - 20\mu^5,$$
$$\varphi_{4,0} = -30\mu^2 + 273\mu^3 - 486\mu^4 + 273\mu^5 - 30\mu^6,$$
$$\varphi_{3,1} = 6\mu - 438\mu^2 + 2604\mu^3 - 4326\mu^4 + 2604\mu^5 - 438\mu^6 + 6\mu^7,$$
$$\varphi_{2,2} = 45\mu - 1665\mu^2 + 8688\mu^3 - 14076\mu^4 + 8688\mu^5 - 1665\mu^6 + 45\mu^7,$$
$$\varphi_{1,3} = 60\mu - 2220\mu^2 + 11796\mu^3 - 19290\mu^4 + 11796\mu^5 - 2220\mu^6 + 60\mu^7,$$

$$\varphi_{0,4} = 15\mu - 885\mu^2 + 5265\mu^3 - 8757\mu^4 + 5265\mu^5 - 885\mu^6 + 15\mu^7,$$
$$\varphi_{5,0} = 15\mu^2 - 600\mu^3 + 3351\mu^4 - 5526\mu^5 + 3351\mu^6 - 600\mu^7 + 15\mu^8,$$
$$\varphi_{4,1} = 450\mu^2 - 9180\mu^3 + 40272\mu^4 - 62964\mu^5 + 40272\mu^6 - 9180\mu^7 + 450\mu^8,$$
$$\varphi_{3,2} = -15\mu + 3165\mu^2 - 46713\mu^3 + 183693\mu^4 - 280209\mu^5 + 183693\mu^6 - 46713\mu^7 + 3165\mu^8 - 15\mu^9,$$
$$\varphi_{2,3} = -60\mu + 7710\mu^2 - 103542\mu^3 + 395046\mu^4 - 597504\mu^5 + 395046\mu^6 - 103542\mu^7 + 7710\mu^8 - 60\mu^9,$$
$$\varphi_{1,4} = -45\mu + 7020\mu^2 - 99855\mu^3 + 391536\mu^4 - 597459\mu^5 + 391536\mu^6 - 99855\mu^7 + 7020\mu^8 - 45\mu^9,$$
$$\varphi_{0,5} = -6\mu + 1926\mu^2 - 32796\mu^3 + 136962\mu^4 - 211938\mu^5 + 136962\mu^6 - 32796\mu^7 + 1926\mu^8 - 6\mu^9.$$

Low-temperature polynomials for the s.c. lattice:

$$g_1(u, v) = u^3v^6,$$
$$g_2(u, v) = u^6(-9\tfrac{1}{2}v^{12} + 6v^{11}) + 3u^5v^{12},$$
$$g_3(u, v) = u^9(151\tfrac{1}{3}v^{18} - 180v^{17} + 42v^{16} + 8v^{15}) + u^8(-84v^{18} + 48v^{17}) + u^7(3v^{18} + 12v^{17}),$$
$$\begin{aligned} g_4(u, v) = {} & u^{12}(-2997\tfrac{3}{4}v^{24} + 5190v^{23} - 2526v^{22} + 22v^{21} + 123v^{20} + 24v^{19} + 2v^{18}) \\ & + u^{11}(2337v^{24} - 2616v^{23} + 612v^{22} + 72v^{21}) + u^{10}(-286\tfrac{1}{2}v^{24} - 276v^{23} + 210v^{22} + 24v^{21}) \\ & + u^9(3v^{24} + 24v^{23} + 48v^{22} + 8v^{21}) + 3u^8v^{22}, \end{aligned}$$
$$\begin{aligned} g_5(u, v) = {} & u^{15}(67082\tfrac{1}{5}v^{30} - 152172v^{29} + 113628v^{28} - 22208v^{27} - 5874v^{26} + 408v^{25} + 416v^{24} + 96v^{23} + 30v^{22}) \\ & + u^{14}(-66972v^{30} + 111120v^{29} - 53664v^{28} + 2760v^{27} + 1884v^{26} + 240v^{25} + 24v^{24}) \\ & + u^{13}(14778v^{30} - 2256v^{29} - 9942v^{28} + 2112v^{27} + 732v^{26} + 108v^{25}) \\ & + u^{12}(-588v^{30} - 2520v^{29} - 768v^{28} + 752v^{27} + 288v^{26} + 24v^{25} + 8v^{24}) \\ & + u^{11}(3v^{30} + 36v^{29} + 36v^{28} + 264v^{27} + 75v^{26} + 12v^{25}) + u^{10}(24v^{27} + 24v^{26}). \end{aligned}$$

High-temperature polynomials for the f.c.c. lattice:

$$\varphi_{0,0} = 1,$$
$$\varphi_{1,0} = -6\mu,$$
$$\varphi_{0,1} = -3\mu,$$
$$\varphi_{2,0} = 15\mu - 21\mu^2 + 15\mu^3,$$
$$\varphi_{1,1} = 18\mu - 18\mu^2 + 18\mu^3,$$
$$\varphi_{0,2} = 3\mu - 6\mu^2 + 3\mu^3,$$
$$\varphi_{3,0} = -20\mu + 230\mu^2 - 414\mu^3 + 230\mu^4 - 20\mu^5,$$
$$\varphi_{1,2} = -18\mu + 180\mu^2 - 324\mu^3 + 180\mu^4 - 18\mu^5,$$
$$\varphi_{2,1} = -45\mu + 369\mu^2 - 663\mu^3 + 369\mu^4 - 45\mu^5,$$
$$\varphi_{0,3} = -\mu + 25\mu^2 - 49\mu^3 + 25\mu^4 - \mu^5,$$
$$\varphi_{4,0} = 15\mu - 885\mu^2 + 5265\mu^3 - 8757\mu^4 + 5265\mu^5 - 885\mu^6 + 15\mu^7,$$
$$\varphi_{3,1} = 60\mu - 2220\mu^2 + 11604\mu^3 - 18858\mu^4 + 11604\mu^5 - 2220\mu^6 + 60\mu^7,$$
$$\varphi_{2,2} = 45\mu - 1665\mu^2 + 8796\mu^3 - 14328\mu^4 + 8796\mu^5 - 1665\mu^6 + 45\mu^7,$$
$$\varphi_{1,3} = 6\mu - 438\mu^2 + 2688\mu^3 - 4506\mu^4 + 2688\mu^5 - 438\mu^6 + 6\mu^7,$$
$$\varphi_{0,4} = -30\mu^2 + 273\mu^3 - 486\mu^4 + 273\mu^5 - 30\mu^6,$$
$$\varphi_{5,0} = -6\mu + 1926\mu^2 - 32796\mu^3 + 136962\mu^4 - 211938\mu^5 + 136962\mu^6 - 32796\mu^7 + 1926\mu^8 - 6\mu^9,$$
$$\varphi_{4,1} = -45\mu + 7020\mu^2 - 98415\mu^3 + 381174\mu^4 - 579123\mu^5 + 381174\mu^6 - 98415\mu^7 + 7020\mu^8 - 45\mu^9,$$
$$\varphi_{3,2} = -60\mu + 7710\mu^2 - 103638\mu^3 + 396150\mu^4 - 600012\mu^5 + 396150\mu^6 - 103638\mu^7 + 7710\mu^8 - 60\mu^9,$$
$$\varphi_{2,3} = -15\mu + 3165\mu^2 - 47805\mu^3 + 191025\mu^4 - 292569\mu^5 + 191025\mu^6 - 47805\mu^7 + 3165\mu^8 - 15\mu^9,$$
$$\varphi_{1,4} = 450\mu^2 - 9432\mu^3 + 42210\mu^4 - 66456\mu^5 + 42210\mu^6 - 9432\mu^7 + 450\mu^8,$$
$$\varphi_{0,5} = 15\mu^2 - 600\mu^3 + 3351\mu^4 - 5526\mu^5 + 3351\mu^6 - 600\mu^7 + 15\mu^8.$$

Low-temperature polynomials for the f.c.c. lattice:

$$g_1(u, v) = u^6v^3,$$
$$g_2(u, v) = u^{12}(-9\tfrac{1}{2}v^6 + 3v^5) + 6u^{11}v^6,$$
$$g_3(u, v) = u^{18}(151\tfrac{1}{3}v^9 - 96v^8 + 15v^7) + u^{17}(-168v^9 + 48v^8) + u^{16}(30v^9 + 12v^8) + 8u^{15}v^9,$$
$$\begin{aligned} g_4(u, v) = {} & u^{24}(-3005\tfrac{3}{4}v^{12} + 2865v^{11} - 889\tfrac{1}{2}v^{10} + 83v^9 + 3v^8) + u^{23}(4698v^{12} - 2772v^{11} + 396v^{10}) \\ & + u^{22}(-1827v^{12} + 36v^{11} + 138v^{10}) + u^{21}(-114v^{12} + 216v^{11} + 24v^{10}) \\ & + u^{20}(72v^{12} + 48v^{11} + 3v^{10}) + u^{19}(12v^{12} + 12v^{11}) + 2u^{18}v^{12}, \end{aligned}$$

$$g_5(u,v) = u^{30}(67528\tfrac{1}{5}v^{15} - 85884v^{14} + 39996v^{13} - 7712v^{12} + 327v^{11} + 48v^{10})$$
$$+ u^{29}(-135516v^{15} + 122040v^{14} - 35568v^{13} + 3192v^{12} + 60v^{11})$$
$$+ u^{28}(81888v^{15} - 31080v^{14} - 2790v^{13} + 1236v^{12} + 36v^{11})$$
$$+ u^{27}(-8184v^{15} - 10896v^{14} + 2400v^{13} + 384v^{12})$$
$$+ u^{26}(-4506v^{15} + 540v^{14} + 1020v^{13} + 72v^{12} + 3v^{11}) + u^{25}(96v^{15} + 360v^{14} + 312v^{13} + 24v^{12})$$
$$+ u^{24}(52v^{15} + 240v^{14} + 156v^{13}) + u^{23}(48v^{15} + 48v^{14}) + u^{22}(24v^{14} + 6v^{13}).$$

High-temperature polynomials for the b.c.c. lattice:

$$\varphi_{0,0} = 1,$$
$$\varphi_{1,0} = -4\mu,$$
$$\varphi_{0,1} = -3\mu,$$
$$\varphi_{2,0} = 6\mu - 10\mu^2 + 6\mu^3,$$
$$\varphi_{1,1} = 12\mu - 12\mu^2 + 12\mu^3,$$
$$\varphi_{0,2} = 3\mu - 6\mu^2 + 3\mu^3,$$
$$\varphi_{3,0} = -4\mu + 64\mu^2 - 120\mu^3 + 64\mu^4 - 4\mu^5,$$
$$\varphi_{2,1} = -18\mu + 162\mu^2 - 282\mu^3 + 162\mu^4 - 18\mu^5,$$
$$\varphi_{1,2} = -12\mu + 120\mu^2 - 216\mu^3 + 120\mu^4 - 12\mu^5,$$
$$\varphi_{0,3} = -\mu + 25\mu^2 - 49\mu^3 + 25\mu^4 - \mu^5,$$
$$\varphi_{4,0} = \mu - 133\mu^2 + 961\mu^3 - 1647\mu^4 + 961\mu^5 - 133\mu^6 + \mu^7,$$
$$\varphi_{3,1} = 12\mu - 588\mu^2 + 3228\mu^3 - 5304\mu^4 + 3228\mu^5 - 588\mu^6 + 12\mu^7,$$
$$\varphi_{2,2} = 18\mu - 714\mu^2 + 3792\mu^3 - 6156\mu^4 + 3792\mu^5 - 714\mu^6 + 18\mu^7,$$
$$\varphi_{1,3} = 4\mu - 292\mu^2 + 1792\mu^3 - 3004\mu^4 + 1792\mu^5 - 292\mu^6 + 4\mu^7,$$
$$\varphi_{0,4} = -30\mu^2 + 273\mu^3 - 486\mu^4 + 273\mu^5 - 30\mu^6,$$
$$\varphi_{5,0} = 140\mu^2 - 3420\mu^3 + 16284\mu^4 - 25964\mu^5 + 16284\mu^6 - 3420\mu^7 + 140\mu^8,$$
$$\varphi_{4,1} = -3\mu + 1023\mu^2 - 16803\mu^3 + 68721\mu^4 - 105741\mu^5 + 68721\mu^6 - 16803\mu^7 + 1023\mu^8 - 3\mu^9,$$
$$\varphi_{3,2} = -12\mu + 1992\mu^2 - 28272\mu^3 + 109740\mu^4 - 166896\mu^5 + 109740\mu^6 - 28272\mu^7 + 1992\mu^8 - 12\mu^9,$$
$$\varphi_{2,3} = -6\mu + 1346\mu^2 - 20586\mu^3 + 82206\mu^4 - 125682\mu^5 + 82206\mu^6 - 20586\mu^7 + 1346\mu^8 - 6\mu^9,$$
$$\varphi_{1,4} = 300\mu^2 - 6288\mu^3 + 28140\mu^4 - 44304\mu^5 + 28140\mu^6 - 6288\mu^7 + 300\mu^8,$$
$$\varphi_{0,5} = 15\mu^2 - 600\mu^3 + 3351\mu^4 - 5526\mu^5 + 3351\mu^6 - 600\mu^7 + 15\mu^8.$$

Low-temperature polynomials for the b.c.c. lattice:

$$g_1(u,v) = u^4v^3,$$
$$g_2(u,v) = u^8(-7\tfrac{1}{2}v^6 + 3v^5) + 4u^7v^6,$$
$$g_3(u,v) = u^{12}(93\tfrac{1}{3}v^9 - 72v^8 + 15v^7) + u^{11}(-88v^9 + 24v^8) + u^{10}(16v^9 + 12v^8),$$
$$g_4(u,v) = u^{16}(-1440\tfrac{3}{4}v^{12} + 1635v^{11} - 646\tfrac{1}{2}v^{10} + 83v^9 + 3v^8)$$
$$+ u^{15}(1920v^{12} - 1152v^{11} + 180v^{10}) + u^{14}(-714v^{12} - 180v^{11} + 96v^{10})$$
$$+ u^{13}(72v^{12} + 96v^{11} + 36v^{10}) + u^{12}(6v^{11} + 6v^{10}).$$
$$g_5(u,v) = u^{20}(25096\tfrac{1}{5}v^{15} - 37524v^{14} + 21666v^{13} - 5484v^{12} + 372v^{11} + 48v^{10})$$
$$+ u^{19}(-43064v^{15} + 40584v^{14} - 13104v^{13} + 1376v^{12} + 24v^{11})$$
$$+ u^{18}(24204v^{15} - 3936v^{14} - 3444v^{13} + 744v^{12} + 24v^{11}) + u^{17}(-5184v^{15} - 4248v^{14} + 360v^{12})$$
$$+ u^{16}(354v^{15} + 468v^{14} + 294v^{13} + 140v^{12} + 6v^{11}) + u^{15}(48v^{14} + 120v^{13} + 48v^{12}) + 12u^{14}v^{12}.$$

High-temperature polynomials of the s.q. lattice:

$$\varphi_{0,0} = 1,$$
$$\varphi_{1,0} = -2\mu,$$
$$\varphi_{0,1} = -2\mu,$$
$$\varphi_{2,0} = \mu - 3\mu^2 + \mu^3,$$
$$\varphi_{1,1} = 4\mu - 4\mu^2 + 4\mu^3,$$
$$\varphi_{0,2} = \mu - 3\mu^2 + \mu^3,$$
$$\varphi_{3,0} = 6\mu^2 - 14\mu^3 + 6\mu^4,$$
$$\varphi_{2,1} = -2\mu + 26\mu^2 - 42\mu^3 + 26\mu^4 - 2\mu^5,$$
$$\varphi_{1,2} = -2\mu + 26\mu^2 - 46\mu^3 + 26\mu^4 - 2\mu^5,$$
$$\varphi_{0,3} = 6\mu^2 - 14\mu^3 + 6\mu^4,$$
$$\varphi_{4,0} = -2\mu^2 + 42\mu^3 - 84\mu^4 + 42\mu^5 - 2\mu^6,$$

$$\varphi_{3,1} = -32\mu^2 + 224\mu^3 - 372\mu^4 + 224\mu^5 - 32\mu^6,$$
$$\varphi_{2,2} = \mu - 65\mu^2 + 377\mu^3 - 615\mu^4 + 377\mu^5 - 65\mu^6 + \mu,$$
$$\varphi_{1,3} = -32\mu^2 + 240\mu^3 - 412\mu^4 + 240\mu^5 - 32\mu^6,$$
$$\varphi_{0,4} = -2\mu^2 + 42\mu^3 - 84\mu^4 + 42\mu^5 - 2\mu^6,$$
$$\varphi_{5,0} = -34\mu^3 + 320\mu^4 - 580\mu^5 + 320\mu^6 - 34\mu^7,$$
$$\varphi_{4,1} = 10\mu^2 - 412\mu^3 + 2096\mu^4 - 3352\mu^5 + 2096\mu^6 - 412\mu^7 + 10\mu^8,$$
$$\varphi_{3,2} = 60\mu^2 - 1160\mu^3 + 4912\mu^4 - 7602\mu^5 + 4912\mu^6 - 1160\mu^7 + 60\mu^8,$$
$$\varphi_{2,3} = 60\mu^2 - 1200\mu^3 + 5184\mu^4 - 8038\mu^5 + 5184\mu^6 - 1200\mu^7 + 60\mu^8,$$
$$\varphi_{1,4} = 10\mu^2 - 436\mu^3 + 2338\mu^4 - 3816\mu^5 + 2338\mu^6 - 436\mu^7 + 10\mu^8,$$
$$\varphi_{0,5} = -34\mu^3 + 320\mu^4 - 580\mu^5 + 320\mu^6 - 34\mu^7,$$
$$\varphi_{6,0} = 8\mu^3 - 423\mu^4 + 2591\mu^5 - 4365\mu^6 + 2591\mu^7 - 423\mu^8 + 8\mu^9,$$
$$\varphi_{5,1} = 280\mu^3 - 4948\mu^4 + 20276\mu^5 - 31096\mu^6 + 20276\mu^7 - 4948\mu^8 + 280\mu^9,$$
$$\varphi_{4,2} = -18\mu^2 + 1562\mu^3 - 17395\mu^4 + 60976\mu^5 - 90154\mu^6 + 60976\mu^7 - 17395\mu^8 + 1562\mu^9 - 18\mu^{10},$$
$$\varphi_{3,3} = -48\mu^2 + 2672\mu^3 - 26724\mu^4 + 90212\mu^5 - 132124\mu^6 + 90212\mu^7 - 26724\mu^8 + 2672\mu^9 - 48\mu^{10},$$
$$\varphi_{2,4} = -18\mu^2 + 1642\mu^3 - 18962\mu^4 + 67776\mu^5 - 100638\mu^6 + 67776\mu^7 - 18962\mu^8 + 1642\mu^9 - 18\mu^{10},$$
$$\varphi_{1,5} = 296\mu^3 - 5484\mu^4 + 23368\mu^5 - 36344\mu^6 + 23368\mu^7 - 5484\mu^8 + 296\mu^9,$$
$$\varphi_{0,6} = 8\mu^3 - 423\mu^4 + 2591\mu^5 - 4365\mu^6 + 2591\mu^7 - 423\mu^8 + 8\mu^9.$$

Low-temperature polynomials for the s.q. lattice:

$$g_1(u, v) = u^2v^2,$$
$$g_2(u, v) = u^4(-4\tfrac{1}{2}v^4 + 2v^3) + 2u^3v^4,$$
$$g_3(u, v) = u^6(32\tfrac{1}{3}v^6 - 28v^5 + 6v^4) + u^5(-24v^6 + 8v^5) + u^4(2v^6 + 4v^5),$$
$$\begin{aligned} g_4(u, v) = {} & u^8(-283\tfrac{1}{4}v^8 + 362v^7 - 150v^6 + 18v^5 + v^4) + u^7(290v^8 - 208v^7 + 36v^6) \\ & + u^6(-61v^8 - 44v^7 + 20v^6) + u^5(2v^8 + 8v^7 + 8v^6) + u^4v^6, \end{aligned}$$
$$\begin{aligned} g_5(u, v) = {} & u^{10}(2771\tfrac{1}{5}v^{10} - 4672v^9 + 2866v^8 - 712v^7 + 34v^6 + 8v^5) \\ & + u^9(-3604v^{10} + 4008v^9 - 1432v^8 + 152v^7 + 4v^6) \\ & + u^8(1238v^{10} + 52v^9 - 456v^8 + 88v^7 + 4v^6) + u^7(-112v^{10} - 272v^9 - 64v^8 + 48v^7) \\ & + u^6(2v^{10} + 12v^9 + 12v^8 + 16v^7 + v^6) + 8u^5v^7, \end{aligned}$$
$$\begin{aligned} g_6(u, v) = {} & u^{12}(-29096\tfrac{1}{2}v^{12} + 60860v^{11} - 49464v^{10} + 18768\tfrac{2}{3}v^9 - 2818v^8 - 82v^7 + 40v^6 + 2v^5) \\ & + u^{11}(45830v^{12} - 69224v^{11} + 37880v^{10} - 8480v^9 + 466v^8 + 48v^7) \\ & + u^{10}(-21920v^{12} + 10872v^{11} + 4804v^{10} - 3232v^9 + 296v^8 + 36v^7) \\ & + u^9(3572\tfrac{2}{3}v^{12} + 4760v^{11} - 1660v^{10} - 920v^9 + 224v^8 + 16v^7) \\ & + u^8(-178v^{12} - 764v^{11} - 724v^{10} - 80v^9 + 87v^8 + 8v^7) + u^7(2v^{12} + 16v^{11} + 20v^{10} - 72v^9 + 64v^8) \\ & + u^6(8v^9 + 28v^8 + 4v^7) + 2u^5v^8. \end{aligned}$$

High-temperature polynomials for the Δ'^r lattice:

$$\varphi_{0,0} = 1,$$
$$\varphi_{1,0} = -3\mu,$$
$$\varphi_{0,1} = -3\mu,$$
$$\varphi_{2,0} = 3\mu - 6\mu^2 + 3\mu^3,$$
$$\varphi_{1,1} = 9\mu - 9\mu^2 + 9\mu^3,$$
$$\varphi_{0,2} = 3\mu - 6\mu^2 + 3\mu^3,$$
$$\varphi_{3,0} = -\mu + 25\mu^2 - 47\mu^3 + 25\mu^4 - \mu^5,$$
$$\varphi_{2,1} = -9\mu + 90\mu^2 - 156\mu^3 + 90\mu^4 - 9\mu^5,$$
$$\varphi_{1,2} = -9\mu + 90\mu^2 - 162\mu^3 + 90\mu^4 - 9\mu^5,$$
$$\varphi_{0,3} = -\mu + 25\mu^2 - 47\mu^3 + 25\mu^4 - \mu^5,$$
$$\varphi_{4,0} = -30\mu^2 + 261\mu^3 - 456\mu^4 + 261\mu^5 - 30\mu^6,$$
$$\varphi_{3,1} = 3\mu - 219\mu^2 + 1284\mu^3 - 2115\mu^4 + 1284\mu^5 - 219\mu^6 + 3\mu^7,$$
$$\varphi_{2,2} = 9\mu - 387\mu^2 + 2103\mu^3 - 3429\mu^4 + 2103\mu^5 - 387\mu^6 + 9\mu^7,$$
$$\varphi_{1,3} = 3\mu - 219\mu^2 + 1326\mu^3 - 2223\mu^4 + 1326\mu^5 - 219\mu^6 + 3\mu^7,$$
$$\varphi_{0,4} = -30\mu^2 + 261\mu^3 - 456\mu^4 + 261\mu^5 - 30\mu^6,$$
$$\varphi_{5,0} = 15\mu^2 - 570\mu^3 + 3072\mu^4 - 5004\mu^5 + 3072\mu^6 - 570\mu^7 + 15\mu^8,$$
$$\varphi_{4,1} = 225\mu^2 - 4482\mu^3 + 19278\mu^4 - 29946\mu^5 + 19278\mu^6 - 4482\mu^7 + 225\mu^8,$$
$$\varphi_{3,2} = -3\mu + 723\mu^2 - 11094\mu^3 + 44079\mu^4 - 67287\mu^5 + 44079\mu^6 - 11094\mu^7 + 723\mu^8 - 3\mu^9,$$

$$\varphi_{2,3} = -3\mu + 723\mu^2 - 11262\mu^3 + 45333\mu^4 - 69447\mu^5 + 45333\mu^6 - 11262\mu^7 + 723\mu^8 - 3\mu^9,$$
$$\varphi_{1,4} = 225\mu^2 - 4608\mu^3 + 20385\mu^4 - 32022\mu^5 + 20385\mu^6 - 4608\mu^7 + 225\mu^8,$$
$$\varphi_{0,5} = 15\mu^2 - 570\mu^3 + 3072\mu^4 - 5004\mu^5 + 3072\mu^6 - 570\mu^7 + 15\mu^8.$$

Low-temperature polynomials for the Δ'^r lattice:

$$g_1(u, v) = u^3v^3,$$
$$g_2(u, v) = u^6(-6\tfrac{1}{2}v^6 + 3v^5) + 3u^5v^6,$$
$$g_3(u, v) = u^9(68\tfrac{1}{3}v^9 - 60v^8 + 9v^7 + 2v^6) + u^8(-54v^9 + 24v^8) + u^7(3v^9 + 6v^8) + 2u^6v^9,$$
$$g_4(u, v) = u^{12}(-878\tfrac{1}{4}v^{12} + 1128v^{11} - 373\tfrac{1}{2}v^{10} - 21v^9 + 12v^8 + 3v^7) + u^{11}(963v^{12} - 825v^{11} + 132v^{10} + 18v^9) + u^{10}(-175\tfrac{1}{2}v^{12} - 60v^{11} + 51v^{10} + 6v^9) + u^9(-39v^{12} + 30v^{11} + 12v^{10} + 2v^9) + 12u^8v^{11} + 3u^7v^{11},$$
$$g_5(u, v) = u^{15}(12623\tfrac{1}{5}v^{15} - 21300v^{14} + 11106v^{13} - 960v^{12} - 495v^{11} - 30v^{10} + 21v^9 + 6v^8) + u^{14}(-17616v^{15} + 22230v^{14} - 7560v^{13} - 72v^{12} + 192v^{11} + 30v^{10}) + u^{13}(5667v^{15} - 2070v^{14} - 1254v^{13} + 198v^{12} + 84v^{11} + 12v^{10}) + u^{12}(456v^{15} - 1374v^{14} + 96v^{13} + 112v^{12} + 24v^{11} + 6v^{10}) + u^{11}(-159v^{15} - 222v^{14} + 150v^{13} + 36v^{12} + 18v^{11}) + u^{10}(-60v^{14} + 78v^{13}) + u^9(15v^{13} + 6v^{12}) + 6u^8v^{13}.$$

APPENDIX B

Listed below are the low-temperature polynomials $g_s(u, v)$ for the third equivalent neighbor model lattices.

s.c.(1, 2, 3) *lattice:*

$$g_1(u) = u^{13},$$
$$g_2(u) = 13u^{25} - 13\tfrac{1}{2}u^{26},$$
$$g_3(u) = 44u^{36} + 193u^{37} - 544u^{38} + 307\tfrac{1}{3}u^{39},$$
$$g_4(u) = 67u^{46} + 288u^{47} + 1263u^{48} + 1189u^{49} - 16336\tfrac{1}{2}u^{50} + 22251u^{51} - 8721\tfrac{3}{4}u^{52},$$
$$g_5(u) = 56u^{55} + 192u^{56} + 1251u^{57} + 3292u^{58} + 8112u^{59} + 15912u^{60} - 60003u^{61} - 356148u^{62} + 1037346u^{63} - 929860u^{64} + 279850\tfrac{1}{5}u^{65}.$$

f.c.c.(1, 2, 3) *lattice:*

$$g_1(u) = u^{21},$$
$$g_2(u) = 21u^{41} - 21\tfrac{1}{2}u^{42},$$
$$g_3(u) = 124u^{60} + 489u^{61} - 1392u^{62} + 779\tfrac{1}{3}u^{63},$$
$$g_4(u) = 333u^{78} + 1320u^{79} + 5709u^{80} + 3341u^{81} - 65926\tfrac{1}{2}u^{82} + 90459u^{83} - 35235\tfrac{3}{4}u^{84}.$$

b.c.c.(1, 2, 3) *lattice:*

$$g_1(u) = u^{13},$$
$$g_2(u) = 13u^{25} - 13\tfrac{1}{2}u^{26},$$
$$g_3(u) = 44u^{36} + 193u^{37} - 544u^{38} + 307\tfrac{1}{3}u^{39},$$
$$g_4(u) = 57u^{46} + 288u^{47} + 1353u^{48} + 1029u^{49} - 16246\tfrac{1}{2}u^{50} + 22251u^{51} - 8731\tfrac{3}{4}u^{52},$$
$$g_5(u) = 28u^{55} + 236u^{56} + 867u^{57} + 3844u^{58} + 8732u^{59} + 18000u^{60} - 71367u^{61} - 342124u^{62} + 1032114u^{63} - 931080u^{64} + 280750\tfrac{1}{5}u^{65}.$$

Δ'^r(1, 2, 3) *lattice:*

$$g_1(u) = u^9,$$
$$g_2(u) = 9u^{17} - 9\tfrac{1}{2}u^{18},$$
$$g_3(u) = 27u^{24} + 72u^{25} - 243u^{26} + 144\tfrac{1}{3}u^{27},$$
$$g_4(u) = 38u^{30} + 117u^{31} + 375u^{32} - 175u^{33} - 4081\tfrac{1}{2}u^{34} + 6402u^{35} - 2675\tfrac{3}{4}u^{36}.$$
$$g_5(u) = 27u^{35} + 111u^{36} + 324u^{37} + 963u^{38} + 925u^{39} + 828u^{40} - 18861u^{41} - 36806u^{42} + 168471u^{43} - 171408u^{44} + 55426\tfrac{1}{5}u^{45}.$$

s.q.(1, 2, 3) *lattice:*

$$g_1(u) = u^6,$$
$$g_2(u) = 6u^{11} - 6\tfrac{1}{2}u^{12},$$
$$g_3(u) = 10u^{15} + 36u^{16} - 114u^{17} + 68\tfrac{1}{3}u^{18},$$
$$g_4(u) = 6u^{18} + 30u^{19} + 111u^{20} + 22u^{21} - 1389u^{22} + 2100u^{23} - 880\tfrac{1}{4}u^{24},$$
$$g_5(u) = u^{20} + 8u^{21} + 53u^{22} + 134u^{23} + 303u^{24} + 328u^{25} - 3230u^{26} - 10688u^{27} + 39660u^{28} - 39262u^{29} + 12693\tfrac{1}{5}u^{30}.$$

APPENDIX C

The tables below contain the lattice constants of the low-temperature spin configurations on the second and third equivalent neighbor model lattices. Tables XIX and XXI contain connected graphs only; the number of occurrences of a connected graph G is denoted by $N[G]$ (see Sec. II), and the numbers $[G]$ are recorded in the tables. The lattice constants of separated configurations $[G]_N$ are given in Tables XX and XXII, where two numbers are recorded for each figure. The upper entry is equal to $[G]_{N=1}$ and the lower entry is the coefficient of N in $[G]_N$.

TABLE XIX. Low-temperature lattice constants of connected graphs containing up to five spins for the second equivalent neighbor model lattices.

L.T. Graph	f.c.c.(1, 2) $q = 18$	s.c.(1, 2) $q = 18$	b.c.c.(1, 2) $q = 14$	$\Delta(1, 2)$ $q = 12$	s.q.(1, 2) $q = 8$
$C(2, 1)$	9	9	7	6	4
$C(3, 1)$	20	20	12	10	4
$C(3, 2)$	93	93	55	36	16
$C(4, 1)$	17	13	6	5	1
$C(4, 2)$	84	96	42	33	8
$C(4, 3)$	9	9	3	3	1
$C(4, 4)$	420	420	192	108	28
$C(4, 5)$	957	933	427	210	64
$C(4, 6)$	160	152	64	26	8
$C(5, 1)$	24	0	0	0	0
$C(5, 2)$	132	108	24	24	4
$C(5, 3)$	0	36	8	6	0
$C(5, 4)$	0	0	0	0	0
$C(5, 5)$	348	468	156	102	12
$C(5, 6)$	0	0	0	0	0
$C(5, 7)$	216	120	48	30	8
$C(5, 8)$	15	33	6	9	1
$C(5, 9)$	24	44	12	12	0
$C(5, 10)$	6	0	0	0	0
$C(5, 11)$	324	276	96	48	4
$C(5, 12)$	756	852	276	126	20
$C(5, 13)$	1296	1368	480	252	48
$C(5, 14)$	354	384	138	57	8
$C(5, 15)$	252	228	72	36	12
$C(5, 16)$	4332	4212	1488	648	116
$C(5, 17)$	2784	2856	984	372	56
$C(5, 18)$	636	528	156	42	8
$C(5, 19)$	4872	4320	1440	414	88
$C(5, 20)$	93	75	25	3	1
$C(5, 21)$	9657	9369	3307	1224	252

TABLE XX. Low-temperature lattice constants of separated graphs containing up to five spins for the second equivalent neighbor model lattices.

L.T. Graph	f.c.c.(1, 2) $q = 18$	s.c.(1, 2) $q = 18$	b.c.c.(1, 2) $q = 14$	$\Delta(1, 2)$ $q = 12$	s.q.(1, 2) $q = 8$
$S(2, 1)$	−9	−9	−7	−6	−4
	$-9\frac{1}{2}$	$-9\frac{1}{2}$	$-7\frac{1}{2}$	$-6\frac{1}{2}$	$-4\frac{1}{2}$
$S(3, 1)$	−255	−255	−153	−108	−48
	−264	−264	−160	−114	−52
$S(3, 2)$	+142	+142	+86	+62	+28
	$+151\frac{1}{3}$	$+151\frac{1}{3}$	$+93\frac{1}{3}$	$+68\frac{1}{3}$	$+32\frac{1}{3}$
$S(4, 1)$	−696	−704	−324	−214	−56
	−716	−724	−336	−224	−60
$S(4, 2)$	−1731	−1719	−797	−456	−135
	$-1771\frac{1}{2}$	$-1759\frac{1}{2}$	$-821\frac{1}{2}$	−474	−143
$S(4, 3)$	−3624	−3576	−1636	−864	−260
	−3717	−3669	−1691	−900	−276
$S(4, 4)$	+7218	+7182	+3346	+1941	+584
	+7563	+7527	+3555	+2091	+652
$S(4, 5)$	−2814	−2806	−1323	−792	−243
	$-3005\frac{3}{4}$	$-2997\frac{3}{4}$	$-1440\frac{3}{4}$	$-878\frac{1}{4}$	$-283\frac{1}{4}$
$S(5, 1)$	−669	−523	−186	−117	−15
	−686	−536	−192	−122	−16
$S(5, 2)$	−3564	−4056	−1374	−831	−136
	−3648	−4152	−1416	−864	−144
$S(5, 3)$	−426	−396	−111	−78	−20
	−435	−405	−114	−81	−21
$S(5, 4)$	−9240	−9264	−3300	−1758	−308
	−9420	−9444	−3384	−1818	−324
$S(5, 5)$	−19020	−19068	−6672	−2988	−508
	−19440	−19488	−6864	−3096	−536
$S(5, 6)$	+21720	+22028	+7836	+4164	+728
	+22616	+22932	+8256	+4448	+804
$S(5, 7)$	−8004	−7284	−2408	−762	−164
	−8164	−7436	−2472	−788	−172
$S(5, 8)$	−47205	−45333	−16043	−6300	−1300
	−48162	−46266	−16470	−6510	−1364
$S(5, 9)$	−47997	−47109	−16637	−7068	−1408
	−48834	−47946	−17022	−7284	−1472
$S(5, 10)$	+114564	+113202	+40632	+18849	+3769
	+118671	+117297	+42549	+19989	+4112
$S(5, 11)$	+120699	+117723	+41829	+17898	+3660
	+125253	+122229	+43905	+19014	+4000
$S(5, 12)$	−210183	−207963	−75311	−35769	−7304
	−221400	−219144	−80588	−38916	−8276
$S(5, 13)$	+63204	+62766	+23029	+11355	+2368
	$+67528\frac{1}{8}$	$+67082\frac{1}{8}$	$+25096\frac{1}{8}$	$+12623\frac{1}{8}$	$+2771\frac{1}{8}$

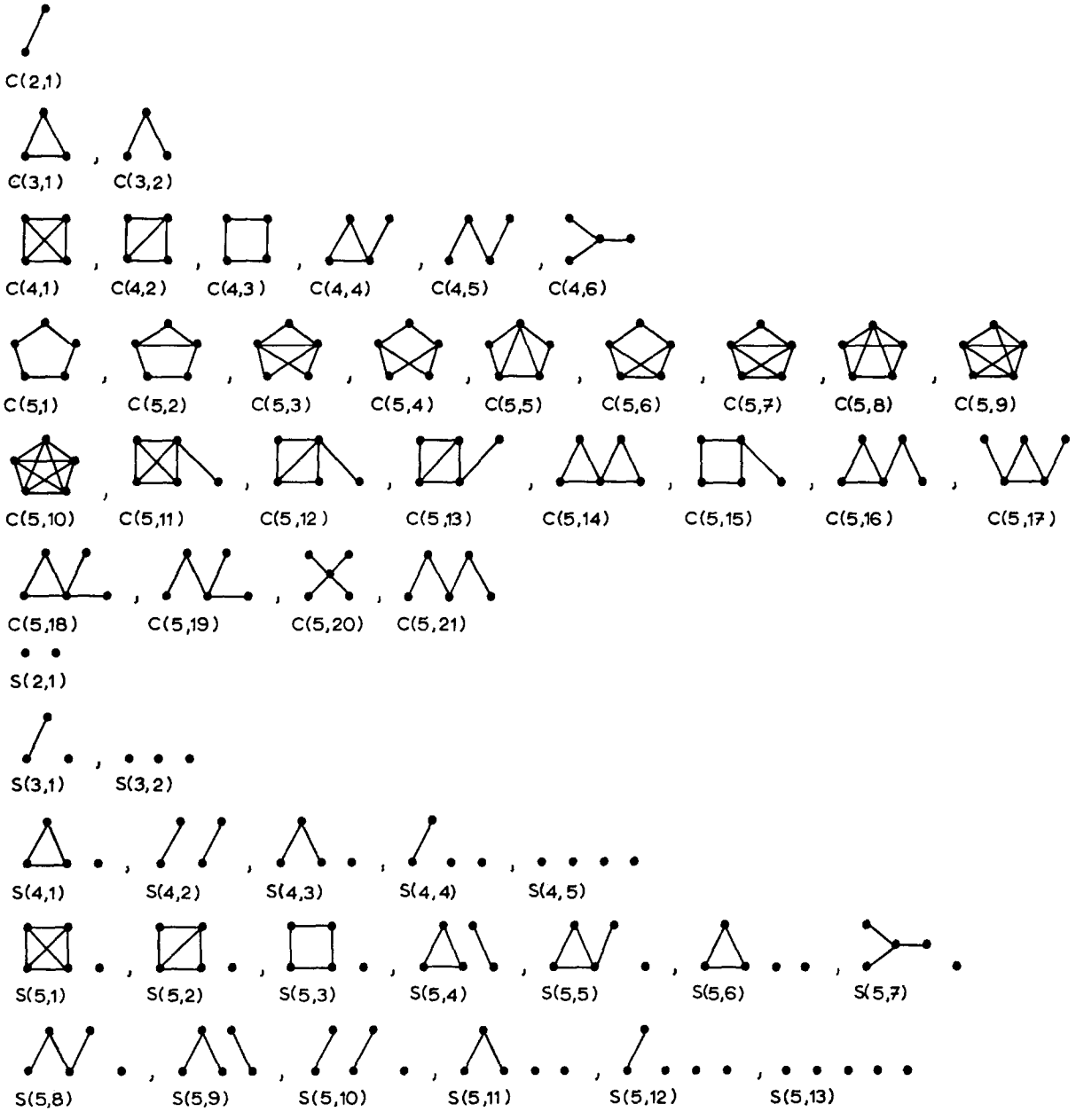
TABLE XXI. Low-temperature lattice constants of connected graphs containing up to five spins for the third equivalent neighbor model lattices.

L.T. Graph	f.c.c.(1, 2, 3) $q = 42$	s.c.(1, 2, 3) $q = 26$	b.c.c.(1, 2, 3) $q = 26$	Δ(1, 2, 3) $q = 18$	s.q.(1, 2, 3) $q = 12$
$C(2, 1)$	21	13	13	9	6
$C(3, 1)$	124	44	44	27	10
$C(3, 2)$	489	193	193	72	36
$C(4, 1)$	333	67	57	38	6
$C(4, 2)$	1320	288	288	117	30
$C(4, 3)$	105	51	21	3	3
$C(4, 4)$	5604	1212	1332	372	108
$C(4, 5)$	11385	2833	2833	606	216
$C(4, 6)$	1904	544	464	58	28
$C(5, 1)$		48	72	12	4
$C(5, 2)$		636	516	42	28
$C(5, 3)$		192	108	18	0
$C(5, 4)$		24	0	0	0
$C(5, 5)$		1380	2028	495	82
$C(5, 6)$		132	0	0	0
$C(5, 7)$		1152	780	312	48
$C(5, 8)$		99	87	12	5
$C(5, 9)$		192	236	111	8
$C(5, 10)$		56	28	27	1
$C(5, 11)$		1588	1708	450	52
$C(5, 12)$		3180	3660	450	116
$C(5, 13)$		6552	6096	1368	252
$C(5, 14)$		1392	1788	336	52
$C(5, 15)$		2292	636	60	44
$C(5, 16)$		18132	19500	3282	664
$C(5, 17)$		10008	12984	1623	350
$C(5, 18)$		3060	2712	186	58
$C(5, 19)$		22440	20136	1458	488
$C(5, 20)$		707	343	3	5
$C(5, 21)$		40957	41173	4953	1258

TABLE XXII. Low-temperature lattice constants of separated graphs containing up to five spins for the third equivalent neighbor model lattices.

L.T. Graph	f.c.c.(1, 2, 3) $q = 42$	s.c.(1, 2, 3) $q = 26$	b.c.c.(1, 2, 3) $q = 26$	Δ(1, 2, 3) $q = 18$	s.q.(1, 2, 3) $q = 12$
$S(2, 1)$	−21	−13	−13	−9	−6
	−21½	−13½	−13½	−9½	−6½
$S(3, 1)$	−1371	−531	−531	−234	−108
	−1392	−544	−544	−243	−114
$S(3, 2)$	+758	+294	+294	+135	+62
	+779⅓	+307⅓	+307⅓	+144⅓	+68⅓
$S(4, 1)$	−9824	−2144	−2224	−812	−212
	−9948	−2188	−2268	−839	−222
$S(4, 2)$	−21489	−5171	−5201	−1449	−459
	−21709½	−5255½	−5285½	−1489½	−477
$S(4, 3)$	−43728	−10888	−10768	−2520	−876
	−44217	−11081	−10961	−2592	−912
$S(4, 4)$	+88626	+21538	+21538	+6078	+1950
	+90459	+22251	+22251	+6402	+2100
$S(4, 5)$	−34236	−8330	−8340	−2491	−794
	−35235¾	−8721¾	−8731¾	−2675¾	−880¼
$S(5, 1)$		−3605	−3271	−1233	−139
		−3672	−3328	−1271	−145
$S(5, 2)$		−17340	−17616	−4218	−762
		−17628	−17904	−4335	−792
$S(5, 3)$		−3516	−1302	−123	−86
		−3567	−1323	−126	−89
$S(5, 4)$		−41008	−42564	−9858	−1756
		−41580	−43136	−10101	−1816
$S(5, 5)$		−77748	−87228	−14676	−2968
		−78960	−88560	−15048	−3076
$S(5, 6)$		+94512	+100020	+22548	+4114
		+97272	+102860	+23630	+4396
$S(5, 7)$		−38924	−32836	−2562	−868
		−39468	−33300	−2620	−896
$S(5, 8)$		−202145	−199985	−26322	−6568
		−204978	−202818	−26928	−6784
$S(5, 9)$		−206465	−206357	−30240	−7188
		−208974	−208866	−30888	−7404
$S(5, 10)$		+490986	+493548	+85830	+19047
		+503229	+505821	+89466	+20190
$S(5, 11)$		+520527	+512823	+75765	+18342
		+534117	+526293	+79005	+19470
$S(5, 12)$		−896715	−897935	−161604	−36106
		−929860	−931080	−171408	−39262
$S(5, 13)$		+267222	+268112	+51495	+11423
		+279850⅕	+280750⅕	+55426⅕	+12693⅕

The connected and separated graphs which are listed in the tables are tabulated below. Each graph is denoted by either $C(x, y)$ (connected) or $S(x, y)$ (separated), where x is the number of vertices of the graph and y serves to identify distinct topological types.



APPENDIX D

The high-temperature ($T > T_c$) expansions of the zero-field susceptibility and zero-field partition function in Eqs. (47) and (48) are most easily derived by using the Van der Waerden identity (for details see Domb[2]), by means of which the series are expressed in ascending powers of $v_1 \{= \tanh(2J_1/kT)\}$ and $v_2 \{= \tanh(2J_2/kT)\}$. The expansion can be put in the form

$$\frac{kT}{m^2}\chi_0 = 1 + 2\sum_{r+s=1}^{\infty} b_{r,s} v_1^r v_2^s,$$

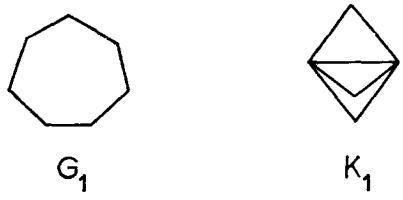
and

$$\log Z = \log 2 + \tfrac{1}{2}q_1 \log\{\cosh(2J_1/kT)\} + \tfrac{1}{2}q_2 \log\{\cosh(2J_2/kT)\} + \sum_{r+s=3}^{\infty} P_{r,s} v_1^r v_2^s,$$

where $b_{r,s}$ and $P_{r,s}$ can be expressed in terms of q_1 and q_2 and the lattice constants of multiply connected diagrams containing n.n. and n.n.n. bonds. These expansions are valid for any regular lattice structure.

Listed below are the coefficients $b_{r,s}$ and $P_{r,s}$ up to orders six and seven, respectively. The coefficients $b_{s,r}$ and $P_{s,r}$ can be obtained from $b_{r,s}$ and $P_{r,s}$ by interchanging q_1 and q_2, and n.n. bonds $C(2, 1)$ with n.n.n. bonds $C_1(2, 1)$. The notation scheme used below to identify the different configurations contributing to the expansion coefficients is fully explained by Dalton.[15]

The only new configurations introduced here are the two diagrams



which contribute to $P_{r,s}$, $r + s = 7$.

The High-Temperature Zero-Field Susceptibility Coefficients $b_{r,s}$

$r + s = 1$:

$$b_{1,0} = \tfrac{1}{2}q_1.$$

$r + s = 2$:

$$b_{2,0} = \tfrac{1}{2}q_1(q_1 - 1),$$
$$b_{1,1} = q_1q_2.$$

$r + s = 3$:

$$b_{3,0} = \tfrac{1}{2}q_1(q_1 - 1)^2 - 3[T_1],$$
$$b_{2,1} = \tfrac{1}{2}q_1q_2(3q_1 - 2) - 3[T_2].$$

$r + s = 4$:

$$b_{4,0} = \tfrac{1}{2}q_1(q_1 - 1)^3 - 4[S_1] - 6(q_1 - 1)[T_1],$$
$$b_{3,1} = q_1q_2(2q_1^2 - 3q_1 + 1) - 4[S_2] - 6q_2[T_1] - (6q_1 - 4)[T_2],$$
$$b_{2,2} = \tfrac{1}{2}q_1q_2(6q_1q_2 - 3q_1 - 3q_2 + 2) - 4\Sigma_2[S_1] - (6q_2 - 2)[T_2] - (6q_1 - 2)[T_3].$$

$r + s = 5$:

$$b_{5,0} = \tfrac{1}{2}q_1(q_1 - 1)^4 - 5[P_1] + 4[F_1] - (8q_1 - 8)[S_1] - (9q_1^2 - 18q_1 + 6)[T_1],$$
$$b_{4,1} = \tfrac{1}{2}q_1q_2(5q_1^3 - 12q_1^2 + 9q_1 - 2) - 5[P_2] + 4\Sigma_1[F_1] - 8q_2[S_1] - (8q_1 - 6)[S_2] - (18q_1q_2 - 12q_2)[T_1] - (9q_1^2 - 14q_1 + 4)[T_2],$$
$$b_{3,2} = \tfrac{1}{2}(10q_1^3q_2^2 - 12q_1^2q_2^2 - 4q_1^3q_2 + 3q_1q_2^2 + 6q_1^2q_2 - 2q_1q_2) - 5\Sigma_2[P_1] + 4\Sigma_2[F_1] - (8q_2 - 2)[S_2] - (8q_1 - 4)\Sigma_2[S_1] - (9q_2^2 - 6q_2)[T_1] - (18q_1q_2 - 4q_1 - 8q_2)[T_2] - (9q_1^2 - 10q_1 + 2)[T_3].$$

$r + s = 6$:

$$b_{6,0} = \tfrac{1}{2}q_1(q_1 - 1)^5 - 6[H_1] + 4[C_1] + 4[B_1] + 4[A_1] - (10q_1 - 10)[P_1] + (8q_1 + 6)[F_1] - (12q_1^2 - 24q_1 + 8)[S_1] - (12q_1^3 - 36q_1^2 + 30q_1 - 9)[T_1],$$
$$b_{5,1} = (3q_1^2q_2 - q_1q_2)(q_1 - 1)^3 - 6[H_2] + 4\Sigma_1[C_1] + 4\Sigma_1[B_1] + 4\Sigma_1[C_1] - 10q_2[P_1] - (10q_1 - 8)[P_2] + 8q_2[F_1] + 8q_1[F_2] + (8q_1 + 6)[F_3] - (24q_1q_2 - 16q_2)[S_1] - (12q_1^2 - 20q_1 + 6)[S_2] - (36q_2q_1^2 - 54q_1q_2 + 12q_2)[T_1] - (q_1 - 1)(12q_1^2 - 18q_1 + 4)[T_2],$$
$$b_{4,2} = \tfrac{1}{2}q_1q_2(q_1 - 1)(15q_1^2q_2 - 15q_1q_2 - 5q_1^2 + 7q_1 + 3q_2 - 2) - 6\Sigma_2[H_1] + 4\Sigma_2[C_1] + 4\Sigma_2[B_1] + 4\Sigma_2[A_1] - (10q_2 - 2)[P_2] - (10q_1 - 6)\Sigma_2[P_1] + (8q_2 + 6)[F_2] + 8q_2[F_3] + 8q_1[F_4] + (8q_1 + 6)(\Sigma_2[F_1] - [F_4]) - (12q_2^2 - 8q_2)[S_1] - (24q_1q_2 - 12q_2 - 4q_1)[S_2] - (12q_1^2 - 16q_1 + 4)\Sigma_2[S_1] - (36q_1q_2^2 - 18q_1q_2 - 18q_2^2 + 12q_2)[T_1] - (36q_1^2q_2 - 42q_1q_2 - 6q_1^2 + 4q_1 + 8q_2 - 3)[T_2] - (12q_1^3 - 24q_1^2 + 14q_1 - 2)[T_3],$$
$$b_{3,3} = q_1q_2(10q_1^2q_2^2 - 10q_1^2q_2 - 10q_1q_2^2 + 8q_1q_2 + 2q_1^2 + 4q_1q_2 + 2q_2^2 - 3q_1 - 3q_2 + 1) - 6\Sigma_3[H_1] + 4\Sigma_3[C_1] + 4\Sigma_3[B_1] + 4\Sigma_3[A_1] - (10q_2 - 4)\Sigma_2[P_1] - (10q_1 - 4)\Sigma_3[P_1] + (8q_2 + 6)[F_4] + (8q_1 + 6)[F_4'] + 8q_2(\Sigma_2[F_1] - [F_4]) + 8q_1(\Sigma_3[F_1] - [F_4']) - (12q_2^2 - 12q_2 + 2)[S_2] - (12q_1^2 - 12q_1 + 2)[S_2'] - (24q_1q_2 - 8q_1 - 8q_2)\Sigma_2[S_1] - (12q_2^3 - 18q_2^2 + 6q_2)[T_1] - (12q_1^3 - 18q_1^2 + 6q_1)[T_4] - (36q_1q_2^2 - 12q_2^2 - 30q_1q_2 + 8q_2 + 4q_1)[T_2] - (36q_1^2q_2 - 12q_1^2 - 30q_1q_2 + 8q_1 + 4q_2)[T_3].$$

The High-Temperature Zero-Field Partition Function Coefficients $P_{r,s}$

$r+s=3$:

$$P_{3,0}=[T_1],$$
$$P_{2,1}=[T_2].$$

$r+s=4$:

$$P_{4,0}=[S_1],$$
$$P_{3,1}=[S_2],$$
$$P_{2,2}=[S_3]+[S_4].$$

$r+s=5$:

$$P_{5,0}=[P_1],$$
$$P_{4,1}=[P_2],$$
$$P_{3,2}=[P_3]+[P_4].$$

$r+s=6$:

$$P_{6,0}=[H_1]-[F_1]-\tfrac{1}{2}[T_1],$$
$$P_{5,1}=\Sigma_1[H_1]-[F_3],$$
$$P_{4,2}=\Sigma_2[H_1]-[F_5]-[F_6]-[F_7]-[F_2]-\tfrac{1}{2}[T_2],$$
$$P_{3,3}=\Sigma_3[H_1]-[F_4]-[F_4'].$$

$r+s=7$:

$$P_{7,0}=[G_1]-2[K_1]-[B_1]-2[F_1],$$
$$P_{6,1}=\Sigma_1[G_1]-2\Sigma_1[K_1]-[B_3]-[B_4]-[B_5]-2[F_2]-[F_3],$$
$$P_{5,2}=\Sigma_2[G_1]-2\Sigma_2[K_1]-[B_2]-[B_9]-[B_{10}]-[B_{12}]-[B_{13}]-[B_{14}]-[F_3]-[F_4]-[F_7],$$
$$P_{4,3}=\Sigma_3[G_1]-2\Sigma_3[K_1]-[B_6]-[B_7]-[B_8]-[B_{21}]-[B_{22}]-[B_{23}]-[B_{24}]-[B_{25}]-[B_{26}]-[F_4]-2[F_5]-2[F_6]-[F_7'].$$

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 7 JULY 1969

Proof of the Symmetrization Postulate

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(Received 22 November 1968)

It is proved within the framework of nonrelativistic quantum mechanics that identical particles are either boson or fermions. The starting assumptions are: (a) if $\psi(x_1\cdots x_n)$ is in the space $\mathcal{K}$ of allowed states, then so is $P\psi$ for every permutation P; (b) $|P\psi|^2=|\psi|^2$ for all $\psi\in\mathcal{K}$, all allowed configurations $(x_1\cdots x_n)$, and all $\psi\in\mathcal{K}$; (c) $\mathcal{K}$ is a vector space (principle of superposition); (d) every $\psi\in\mathcal{K}$ is continuous along every path in the n-particle configuration space $\mathcal{C}$; and (e) there is at least one physical observable connecting each pair of irreducible components of $\mathcal{C}$.

The available observational evidence is all consistent with the postulate, called the *symmetrization postulate* by Messiah,[1,2] that allowed states of a system of identical particles are either all symmetric or all antisymmetric under permutations. Correct proofs of the symmetrization postulate involve not only general properties of physical observables and states of identical particles, but also topological considerations related to the connectivity properties of the configuration space.[3,4] These enter because symmetries more complicated than Bose and Fermi are incompatible with the continuity of allowed wavefunctions along every path in configuration space; a path is connected by definition.

Previous proofs were restricted either to systems with spatially-connected configuration spaces[3] or to particles without spin or other internal degrees of freedom.[4] The proof sketched here lifts both of these restrictions.

Consider a system of n identical particles with allowed wavefunctions $\psi(x_1\cdots x_n)$, where x_j stands for the position $\mathbf{r}_j$ and any internal variables (including spin) of the jth particle. It will be necessary to make use of several lemmas relating to the geometry of configuration space. The *extended one-particle configuration space* $\mathcal{S}_e$ is defined as the set of all x (x stands for a typical x_j). The *forbidden one-particle configuration space* $\mathcal{S}_0$ is the set of all points of $\mathcal{S}_e$ at which *all* allowed ψ vanish (i.e., ψ vanishes when any

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[4] M. Flicker and H. S. Leff, Phys. Rev. **163**, 1353 (1967).

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$$P_{2,2}=[S_3]+[S_4].$$

$r+s=5$:

$$P_{5,0}=[P_1],$$
$$P_{4,1}=[P_2],$$
$$P_{3,2}=[P_3]+[P_4].$$

$r+s=6$:

$$P_{6,0}=[H_1]-[F_1]-\tfrac{1}{2}[T_1],$$
$$P_{5,1}=\Sigma_1[H_1]-[F_3],$$
$$P_{4,2}=\Sigma_2[H_1]-[F_5]-[F_6]-[F_7]-[F_2]-\tfrac{1}{2}[T_2],$$
$$P_{3,3}=\Sigma_3[H_1]-[F_4]-[F_4'].$$

$r+s=7$:

$$P_{7,0}=[G_1]-2[K_1]-[B_1]-2[F_1],$$
$$P_{6,1}=\Sigma_1[G_1]-2\Sigma_1[K_1]-[B_3]-[B_4]-[B_5]-2[F_2]-[F_3],$$
$$P_{5,2}=\Sigma_2[G_1]-2\Sigma_2[K_1]-[B_2]-[B_9]-[B_{10}]-[B_{12}]-[B_{13}]-[B_{14}]-[F_3]-[F_4]-[F_7],$$
$$P_{4,3}=\Sigma_3[G_1]-2\Sigma_3[K_1]-[B_6]-[B_7]-[B_8]-[B_{21}]-[B_{22}]-[B_{23}]-[B_{24}]-[B_{25}]-[B_{26}]-[F_4]-2[F_5]-2[F_6]-[F_7'].$$

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(Received 22 November 1968)

It is proved within the framework of nonrelativistic quantum mechanics that identical particles are either boson or fermions. The starting assumptions are: (a) if $\psi(x_1\cdots x_n)$ is in the space $\mathcal{K}$ of allowed states, then so is $P\psi$ for every permutation P; (b) $|P\psi|^2=|\psi|^2$ for all $\psi\in\mathcal{K}$, all allowed configurations $(x_1\cdots x_n)$, and all $\psi\in\mathcal{K}$; (c) $\mathcal{K}$ is a vector space (principle of superposition); (d) every $\psi\in\mathcal{K}$ is continuous along every path in the n-particle configuration space $\mathcal{C}$; and (e) there is at least one physical observable connecting each pair of irreducible components of $\mathcal{C}$.

The available observational evidence is all consistent with the postulate, called the *symmetrization postulate* by Messiah,[1,2] that allowed states of a system of identical particles are either all symmetric or all antisymmetric under permutations. Correct proofs of the symmetrization postulate involve not only general properties of physical observables and states of identical particles, but also topological considerations related to the connectivity properties of the configuration space.[3,4] These enter because symmetries more complicated than Bose and Fermi are incompatible with the continuity of allowed wavefunctions along every path in configuration space; a path is connected by definition.

Previous proofs were restricted either to systems with spatially-connected configuration spaces[3] or to particles without spin or other internal degrees of freedom.[4] The proof sketched here lifts both of these restrictions.

Consider a system of n identical particles with allowed wavefunctions $\psi(x_1\cdots x_n)$, where x_j stands for the position $\mathbf{r}_j$ and any internal variables (including spin) of the jth particle. It will be necessary to make use of several lemmas relating to the geometry of configuration space. The *extended one-particle configuration space* $\mathcal{S}_e$ is defined as the set of all x (x stands for a typical x_j). The *forbidden one-particle configuration space* $\mathcal{S}_0$ is the set of all points of $\mathcal{S}_e$ at which *all* allowed ψ vanish (i.e., ψ vanishes when any

[1] A. Messiah, *Quantum Mechanics* (North-Holland Publ. Co., Amsterdam, 1962), Vol. II, p. 595.
[2] A. M. L. Messiah and O. Greenberg, Phys. Rev. **136**, B248 (1964).
[3] M. D. Girardeau, Phys. Rev. **139**, B500 (1965).
[4] M. Flicker and H. S. Leff, Phys. Rev. **163**, 1353 (1967).

$x_j \in \mathcal{S}_0$) as a result of constraints or boundary conditions. The *one-particle configuration space* $\mathcal{S} \equiv \mathcal{S}_e - \mathcal{S}_0$. The *distance* between two points in $\mathcal{S}$ is

$$|x - x'| \equiv \left[(\mathbf{r} - \mathbf{r}')^2 + \sum_{j=1}^{\nu}(\tau_j - \tau_j')^2\right]^{\frac{1}{2}} \quad (1)$$

where $\tau_1 \cdots \tau_\nu$ (assumed defined so as to be real) are all internal variables (assumed discrete) included in the one-particle configuration x. The *extended configuration space* $\mathcal{C}_e$ is the set of all ordered n-tuples $X = (x_1 \cdots x_n)$ for which every $x_j \in \mathcal{S}$. The *forbidden configuration space* $\mathcal{C}_0$ is the set of all points of $\mathcal{C}_e$ at which *every* allowed $\psi(X)$ vanishes. $\mathcal{C}_0$ need not be null because of the possibility of two-particle constraints (e.g., hard cores). The *configuration space* $\mathcal{C} \equiv \mathcal{C}_e - \mathcal{C}_0$. The *distance* between two points in $\mathcal{C}$ is

$$|X - X'| \equiv \left[\sum_{j=1}^{n}(|x_j - x_j'|)^2\right]^{\frac{1}{2}}. \quad (2)$$

Lemma 1: $\mathcal{C}_e$, $\mathcal{C}_0$, and $\mathcal{C}$ are all closed under permutations.

Here permutations P are regarded as linear operators in $\mathcal{C}_e$, defined by $X \to PX$ where PX differs from X by a permutation of $x_1 \cdots x_n$. The lemma is a trivial consequence of the previous definitions, provided that $\psi(PX) \in \mathcal{H}$ if and only if $\psi(X) \in \mathcal{H}$; this we assume as part of the definition of identical particles. Here $\mathcal{H}$ is the space of allowed states of the system.

Lemma 2: If $\mathcal{C}$ is not connected, then its connected subspaces $\mathcal{C}_\alpha$ are permuted bodily under the action of the transformations $X \to PX$. $\mathcal{C}_\alpha$ which are images of each other under permutations are congruent in the usual geometrical sense.

This is a consequence of the fact that the permutations are orthogonal operators on $\mathcal{C}$, i.e.,

$$|PX - PX'| = |X - X'|.$$

Divide the set of all $\mathcal{C}_\alpha$ into classes $\mathcal{K}_j$, such that all C_α in a given class are congruent but the $\mathcal{C}_\alpha$ in different classes are not. If all the $\mathcal{C}_\alpha$ in $\mathcal{K}_j$ are images of each other under permutations, then the subspace of $\mathcal{C}$ composed of the union of all $\mathcal{C}_\alpha \in \mathcal{K}_j$ is said to be *irreducible*; otherwise it is *reducible*. Every reducible subspace can be decomposed into irreducible ones.

Lemma 3: $\mathcal{C}$ can be decomposed into irreducible subspaces each of which is either connected or is the union of congruent subspaces each of which is connected.

Lemma 4: Assume the following: (a) if $\psi(x_1 \cdots x_n)$ is in the space $\mathcal{H}$ of allowed states, then so is $P\psi$ for every permutation P, (b) $|P\psi|^2 = |\psi|^2$ for all P, all allowed configurations $(x_1 \cdots x_n)$, and all $\psi \in \mathcal{H}$, (c) $\mathcal{H}$ is a vector space (principle of superposition), (d) every $\psi \in \mathcal{H}$ is continuous along every path in the n-particle configuration space $\mathcal{C}$, and suppose that $\mathcal{C}$ is irreducible. Then either all $\psi \in \mathcal{H}$ are completely symmetric, or else all are completely antisymmetric.

We note first that the same conclusion has already been established[4] for the special case of connected $\mathcal{C}$. This restriction is severe; in particular, it rules out particles with spin or other internal degrees of freedom, as a consequence of (1) and (2). However, the same method of proof shows[3,4] that in the general case

$$P\psi(X) = C_P(X)\psi(X), \quad (3)$$

where

$$C_{QP}(X) = C_Q(X)C_P(X), \quad QC_P(X) = C_P(X). \quad (4)$$

Since $\mathcal{C}$ is irreducible, it consists of congruent connected subspaces $\mathcal{C}_\alpha$ which are all images of each other under appropriate permutations. It follows from the first Eq. (4) that the $C_P(X)$ form a scalar representation of the permutation group at each fixed X, so that $C_P(X) = \pm 1$ at each X. By the definition of $\mathcal{C}$ ($\mathcal{C}_0$ excluded from $\mathcal{C}$), at each $X \in \mathcal{C}$ there is a $\psi \in \mathcal{H}$ such that $\psi(X) \neq 0$. If $C_P(X)$ jumped from $+1$ to -1 at the point $X \in \mathcal{C}_\alpha$, the wavefunction $P\psi \in \mathcal{H}$ would be discontinuous at X, contradicting hypothesis (d). Hence $C_P(X)$ is constant in each $\mathcal{C}_\alpha$:

$$C_P(X) = C_{P,\alpha}, \quad X \in \mathcal{C}_\alpha. \quad (5)$$

By irreducibility of $\mathcal{C}$, for any $X \in \mathcal{C}_\alpha$ and any β there is a permutation Q such that $QX \in \mathcal{C}_\beta$. It then follows from (5) and the second Eq. (4) that $C_{P,\alpha}$ is, in fact, independent of α, i.e.,

$$P\psi(X) = C_P\psi(X) \quad (6)$$

for all $X \in \mathcal{C}$. Since the C_P form a scalar representation of the permutation group, the conclusion of Lemma 4 follows.

Lemma 5: Assume hypotheses (a), (b), (c), and (d). Denote the irreducible subspaces of $\mathcal{C}$ by $\mathcal{C}^\nu$. Then

$$P\psi(X) = C_P^\nu\psi(X), \quad X \in \mathcal{C}^\nu, \quad (7)$$

where, for each fixed ν, C_P^ν is either the Bose representation $C_P^\nu = 1$ (all P) or the Fermi representation $C_P^\nu = (-1)^{p(P)}$.

This follows from Lemmas 3 and 4.

To complete the proof of the symmetrization postulate it is necessary to dispose of the possibility

that the Bose representation might hold in some $\mathcal{C}^\nu$ and the Fermi representation in others. This can be done by making use of properties of physical observables. We note first that every physical observable O commutes with every permutation of identical particles:

$$[O, P] = 0. \tag{8}$$

This is not an additional assumption; it follows[5] from the assumptions[6] that $O\psi \in \mathcal{H}$ if $\psi \in \mathcal{H}$ and that $|P\psi|^2 = |\psi|^2$.

Theorem (*Symmetrization*): Assume hypotheses (a)–(d), and (e) there is at least one physical observable connecting each pair of irreducible components of $\mathcal{C}$ in the sense that, for every pair of irreducible subspaces $\mathcal{C}^\mu$, $\mathcal{C}^\nu$, one assumes the existence of at least one physical observable $O^{\mu\nu}$ which connects $\mathcal{C}^\mu$ and $\mathcal{C}^\nu$ in the sense that

$$O^{\mu\nu}\psi^\nu(X) \neq 0 \text{ for some } \psi^\nu \in \mathcal{H} \text{ and some } X \in \mathcal{C}^\mu, \quad \text{where } \psi^\nu(X) = 0 \text{ for all } X \notin \mathcal{C}^\nu. \tag{9}$$

Then either all $\psi \in \mathcal{H}$ are completely symmetric, or else all are completely antisymmetric.

Note first that

$$PO^{\mu\nu}\psi^\nu(X) = O^{\mu\nu}[P\psi^\nu(X)] = O^{\mu\nu}[C_P^\nu\psi^\nu(X)] = C_P^\nu O^{\mu\nu}\psi^\nu(X), \quad \text{all} \quad X \in \mathcal{C}, \tag{10}$$

where the first equality follows from (8) and the second equality follows from Lemma 5 if $X \in \mathcal{C}^\nu$, and otherwise follows trivially from the vanishing of $\psi^\nu(X)$ [hence, $P\psi^\nu(X)$] if $X \notin \mathcal{C}^\nu$ (recall that $|P\psi^\nu|^2 = |\psi^\nu|^2$). Applying Lemma 5 again with $\psi = O^{\mu\nu}\psi^\nu$ and $X \in \mathcal{C}^\mu$, one has

$$P[O^{\mu\nu}\psi^\nu(X)] = C_P^\mu[O^{\mu\nu}\psi^\nu(X)], \quad X \in \mathcal{C}^\mu. \tag{11}$$

Thus,

$$(C_P^\mu - C_P^\nu)O^{\mu\nu}\psi^\nu(X) = 0, \quad X \in \mathcal{C}^\mu. \tag{12}$$

Then, by (9), $C_P^\mu = C_P^\nu$ for all μ and ν, i.e., $C_P^\mu = C_P$, independent of μ. The theorem then follows by the usual argument (the C_P form a scalar representation of the permutation group).

In order to make the theorem relevant to the real world it is necessary to show that physical observables $O^{\mu\nu}$ satisfying (9) can be found. Note first that such an $O^{\mu\nu}$ can be represented as an integral[7] operator

$$O^{\mu\nu}\psi(X) = \int K^{\mu\nu}(X, X')\psi(X')\,dX' \tag{13}$$

with a kernel $K^{\mu\nu}$ which is nonvanishing when X is in some subspace of $\mathcal{C}^\mu$ and X' in some subspace of $\mathcal{C}^\nu$. The requirement (8) is satisfied by $O^{\mu\nu}$ if

$$K^{\mu\nu}(PX, PX') = K^{\mu\nu}(X, X'). \tag{14}$$

As an example, consider a system of n electrons in a box. Then each irreducible component of $\mathcal{C}$ consists of all configurations with the same value of the z component of total spin angular momentum; there are $2S + 1$ such $\mathcal{C}^\nu$, where $S = \frac{1}{2}n$. The $K^{\mu\nu}$ can then be chosen so that each $O^{\mu\nu}$ is an appropriate power of S_+ or S_- where $S_\pm = S_x \pm iS_y$ and S_x, S_y, S_z are the components of the total spin angular momentum. Eq. (9) is then satisfied for these $O^{\mu\nu}$. It might be objected that if $n \sim 10^{23}$, some of the required $O^{\mu\nu}$ are very high powers of S_+ or S_-, which one might object to regarding as physically observable. However, the proof of the symmetrization theorem could be refined in this case by proving equality of C_P^μ and C_P^ν only for "adjacent" subspaces $\mathcal{C}^\mu$ and $\mathcal{C}^\nu$; equality for all such special choices implies equality for all μ and ν.

It is not possible to give a mathematical proof of the existence of physical observables $O^{\mu\nu}$ satisfying (9) for the case of a completely general system of identical particles. However, such a proof should not be sought; the existence of such $O^{\mu\nu}$ should really be regarded as part of the definition of identical particles. If two subspaces of $\mathcal{C}$ could not be connected by any conceivable physical process, then the particles associated with those subspaces would behave as operationally distinct species.

ACKNOWLEDGMENT

This work was supported by the National Science Foundation under grant GP-7689.

[5] It was shown in the course of a previous proof (see Ref. 3) that $[P\psi_1(X)]^* P\psi_2(X) = \psi_1^*(X)\psi_2(X)$ as a consequence of $|P\psi(X)|^2 = |\psi(X)|^2$ for *all* $\psi \in \mathcal{H}$ and the linearity of $\mathcal{H}$. Take $\psi_1 = P^{-1}\psi_\alpha$, $\psi_2 = O\psi_\beta$ where $\{\psi_\alpha\}$ is any complete orthonormal set. Then straightforward algebra yields $(\psi_\alpha, PO\psi_\beta) = (\psi_\alpha, OP\psi_\beta)$, from which (8) follows.

[6] Strictly speaking, one should only require that $O\psi$ be defined on a dense subset of $\mathcal{H}$. This complicates the analysis but does not change the conclusion (8).

[7] $\int dX$ stands for integration over all spatial variables and summation over (discrete) internal variables.