JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Quantization of the Generalized Hamiltonian

C. F. HAYES
Department of Physics and Astronomy, University of Hawaii, Honolulu, Hawaii

(Received 29 January 1969)

Quantization of systems described by Lagrangians with higher-order derivatives is performed. It is shown that the usual Lagrangian with first-order derivatives may be consistently replaced by one with second-order derivatives, the resulting wavefunction being one of a mixed representation.

I. INTRODUCTION

The Hamilton–Lagrange theory was extended to include higher-order derivatives by Ostrogradsky[1] in 1850. By taking the variation of the time integral of a Lagrangian containing the nth derivative of the generalized coordinates while holding the end points fixed, one obtains the equation of motion. By letting the end points also vary, the generalized momenta are found and, hence, a Hamiltonian which is constant in time for Lagrangians not explicitly time-dependent. It is easily shown that the generalized momenta and the derivatives of the generalized coordinates are related by the Hamilton canonical equations.

In 1940, Bopp[2] and, in 1942, Podolsky,[3] prompted by divergences in electromagnetic theory, proposed Lagrangians containing the second derivative of the potential. Quantization of the theory resulted in finite energies.

The success of these calculations gives rise to several investigations[4] of the quantization of the Ostrogradsky theory. These investigations concerned Bopp and Podolsky's calculations, relativistic effects, and approximations which simplify the Ostrogradsky quantization. Green[5] included another term involving the second derivative of the potential into Podolsky's Lagrangian and obtained a generalized meson-field theory which also led to finite energies. The success of this calculation led Pais and Uhlenbeck,[6] in 1950, to consider if, in general, divergent features of field theory could be eliminated by using higher-order field equations. However, they found no way to reconcile convergence, positive-definite free-field energy, and causality of the state vector.

Subsequently, little work was done on the generalized theory until 1958, when Borneas[7] reasserted the facility of the Ostrogradsky method. This presentation was amplified by Koestler and Smith[8] in 1965 and by Kruger and Callebaut[9] in 1968.

II. OSTROGRADSKY'S THEORY

Ostrogradsky assumed that if a Lagrangian contains derivatives of arbitrarily high but finite order, the appropriate equation of motion will be obtained by setting the variation of the time integral equal to zero. We have

$$\delta\int_{t_1}^{t_2} L(Q_j, DQ_j, D^2Q_j, \cdots, D^NQ_j, t)\,dt = 0, \quad (1)$$

where $j = 1, 2, \cdots, R$ and $D = d/dt$. Holding the end points fixed gives the equations of motion:

$$\sum_{n=0}^{N}(-1)^n D^n\left(\frac{L}{D^nQ_j}\right) = 0. \quad (2)$$

Letting the end points vary gives rise to the generalized momenta:

$$P_{j,n} = \sum_{i=0}^{N-n}(-1)^i D^i\left(\frac{L}{D^{i+n}Q_j}\right), \quad (3)$$

where $n = 1, 2, \cdots, N$. Note that the right side of Eq. (3) is the functional derivative of L with respect to D^nQ_j. If one defines a Hamiltonian analogous to the usual form when no higher derivatives are present, one again obtains a function which is constant if the Lagrangian is not an explicit function of time. We have

$$H = \sum_{j=1}^{R}\sum_{n=1}^{N} P_{j,n}D^nQ_j - L(Q_j, DQ_j, \cdots, D^NQ_j, t). \quad (4)$$

[1] M. Ostrogradsky, Mem. Acad. St. Petersburg 6 (4), 385 (1850); E. T. Whittaker, *Treatise on the Analytical Dynamics of Particles and Rigid Bodies* (Cambridge University Press, Cambridge, England, 1959), 4th ed., p. 266.
[2] F. Bopp, Ann. Physik **38**, 345 (1940).
[3] B. Podolsky, Phys. Rev. **62**, 68 (1942); B. Podolsky and C. Kikuchi, *ibid.* **65**, 228 (1944); **67**, 184 (1945); B. Podolsky and P. Schwed, Rev. Mod. Phys. **20**, 40 (1948).
[4] D. Montgomery, Phys. Rev. **69**, 117 (1946). E. Kanai and S. Takagi, Progr. Theoret. Phys. (Kyoto) **1**, 43 (1946). T. Chang, Proc. Cambridge Phil. Soc. **42**, 132 (1946); **43**, 196 (1947); A. Green, Phys. Rev. **72**, 628 (1947); J. De Wet, Proc. Cambridge Phil. Soc. **44**, 546 (1948).
[5] A. Green, Phys. Rev. **73**, 26 (1948); **75**, 1926 (1949).
[6] A. Pais and G. Uhlenbeck, Phys. Rev. **79**, 145 (1950).
[7] M. Borneas, Am. J. Phys. **27**, 265 (1959); M. Borneas, Nuovo Cimento **16**, 806 (1960).
[8] J. Koestler and J. Smith, Am. J. Phys. **33**, 140 (1965).
[9] J. Kruger and D. Callebaut, Am. J. Phys. **36**, 557 (1968).

It would be desirable to find pairs of canonical variables, but in seeking these we encounter a problem which does not occur in the usual theory. For a given j variable, the Hamiltonian is a function of N momenta, the generalized coordinate, and N derivatives of the generalized coordinate. Obviously, not all of these $2N + 1$ variables can be taken by pairs. This problem is not met in the usual formulation since the highest derivative of the generalized coordinate, the velocity, can be expressed in terms of the momentum. However, for our case we have no guarantee that Eq. (3) will be such that the highest derivative can be expressed in terms of the other $2N$ variables. In fact, in Sec. IV an example is considered where Eq. (3) can not be used. We will find that, rather, the equation of motion (2) must be applied.

The remaining $2N$ variables are easily paired since

$$\frac{\partial H}{\partial P_{j,n}} = \frac{d}{dt}(D^{n-1}Q_j), \tag{5}$$

$$\frac{\partial H}{\partial D^{n-1}Q_j} = -\frac{d}{dt}(P_{j,n}). \tag{6}$$

Thus $P_{j,n}$ and $D^{n-1}Q_j$ act as canonical variables where $n = 1, 2, \cdots, N$.

III. QUANTIZATION

We may define the Poisson bracket, using the generalized variables, to be

$$\{U, V\} = \sum_{j=1}^{R}\sum_{n=1}^{N}\left(\frac{\partial U}{\partial D^{n-1}Q_j}\frac{\partial V}{\partial P_{j,n}} - \frac{\partial U}{\partial P_{j,n}}\frac{\partial V}{\partial D^{n-1}Q_j}\right). \tag{7}$$

Consequently, we find, in analogy to the usual formulation,

$$\{D^{m-1}Q_j, D^{n-1}Q_k\} = \{P_{j,m}, P_{k,n}\} = 0, \tag{8}$$

$$\{D^{m-1}Q_k, P_{j,n}\} = \delta_{kj}\delta_{mn}, \tag{9}$$

$$\{D^{n-1}Q_j, H\} = \frac{\partial H}{\partial P_{j,n}}, \tag{10}$$

$$\{P_{j,n}, H\} = -\frac{\partial H}{\partial D^{n-1}Q_j}. \tag{11}$$

Comparison of Eqs. (10) and (11) with (5) and (6) leads us to seek to quantize the theory. Letting the variables be considered as operators, we postulate

$$[P_{j,n}, D^{m-1}Q_k] = P_{j,n}D^{m-1}Q_k - D^{m-1}Q_kP_{j,n} = \frac{\hbar}{i}C(n, N)\delta_{nm}\delta_{jk}, \tag{12}$$

where $C(n, N)$ is a c number and perhaps a function of n and N.

We take the function F to be any term of H, assumed of the form

$$F = \prod_{j=1}^{R}\prod_{n=0}^{N-1}(P_{j,n})^{a(j,n)}(D^nQ_j)^{b(j,n)}, \tag{13}$$

where $a(j, n)$ and $b(j, n)$ are arbitrary constants. With the use of Eq. (12) one finds

$$[D^{n-1}Q_j, F] = -\frac{\hbar}{i}C(n, N)\frac{\partial F}{\partial P_{j,n}}, \tag{14}$$

$$[P_{j,n}, F] = \frac{\hbar}{i}C(n, N)\frac{\partial F}{\partial D^{n-1}Q_j}, \tag{15}$$

and so

$$[D^{n-1}Q_j, H] = -\frac{\hbar}{i}C(n, H)\frac{\partial H}{\partial P_{j,n}}, \tag{16}$$

$$[P_{j,n}, H] = \frac{\hbar}{i}C(n, N)\frac{\partial H}{\partial D^{n-1}Q_j}. \tag{17}$$

Equations (16) and (17) may be considered the generalized Heisenberg equations of motion for Bose–Einstein quantization. If we let $C(1, 1) = 1$, we find that (16) and (17) reduce to the nongeneralized equations of motion.

For consistency we must demonstrate that one is permitted to choose a c number for the right side of Eq. (12). We must show the commutator of $P_{j,n}$ and $D^{n-1}Q_j$ commutes with H:

$$[[P_{j,n}, D^{n-1}Q_j], H] = i\hbar C(n, N)\left\{\left[P_{j,n}, \frac{\partial H}{\partial P_{j,n}}\right] - \left[\frac{\partial H}{\partial D^{n-1}Q_j}, D^{n-1}Q_j\right]\right\} = 0, \tag{18}$$

where we have used Eqs. (14) and (15) with F being $\partial H/\partial D^{n-1}Q_j$ and $\partial H/\partial P_{j,n}$, respectively.

For completeness we should note that the commutation brackets in Eqs. (12)–(18) may be replaced by anticommutation brackets to obtain a generalized Fermi–Dirac quantization.

The validity of the postulate (12) rests, of course, upon the experimental implications that result. It is for this reason that we have not taken the restriction $C(n, N) = 1$, as is generally done. Actually, to obtain results consistent with experiment, we will note in Sec. V that $C(n, N)$ can not be taken as one in the given example. Although Eq. (12) generalizes the Heisenberg uncertainty relation, we must assert a type of correspondence principle such that if Eq. (12) embodies only the variables of the usual uncertainty relation, $C(n, N)$ must be such that the usual uncertainty relation holds. We will return to this topic in Sec. IV.

If Eq. (12) operates on a wavefunction, one may take

$$P_{j,n} \rightarrow \frac{\hbar}{i} C(n, N) \frac{\partial}{\partial D^{n-1} Q_j} \quad \text{and} \quad D^{m-1} Q_k \rightarrow D^{m-1} Q_k \tag{19}$$

or

$$P_{j,n} \rightarrow P_{j,n} \quad \text{and} \quad D^{m-1} Q_k \rightarrow -\frac{\hbar}{i} C(n, N) \frac{\partial}{\partial P_{k,m}}. \tag{20}$$

These operators may now be used for the wave equation

$$H\Psi_k = E_k \Psi_k, \tag{21}$$

where E_k is the eigenvalue of H. However, we have not shown that E_k corresponds to the energy and, in fact, in general it will not. If H classically is equal to the energy, however, it seems understandable that E_k is the energy eigenvalue.

If Eq. (19) is used, Ψ_k will be a function of Q_j, $DQ_j, \cdots, D^{N-1}Q_j$, with the scalar product defined

$$(\Psi_k, \Psi_{k'}) = \int \prod_{j=1}^{R} dQ_j \, dDQ_j \cdots dD^{N-1}Q_j \Psi_k^* \Psi_{k'}. \tag{22}$$

Equation (20) may be used to give the momentum representation. Also, since Eqs. (19) and (20) hold for each value of n, by using both equations a crossed representation results.

IV. AN ALTERNATIVE TO KINETIC ENERGY IN THE LAGRANGIAN

The usual classical Lagrangian is written as the difference between the kinetic and the potential energies. However, if higher derivatives are permitted, one can have

$$L = -\tfrac{1}{2} \sum_{j=1}^{3} m x_j D^2 x_j - V(x_1, x_2, x_3), \tag{23}$$

which has the required equations of motion

$$m D^2 x_j = -\frac{\partial V}{\partial x_j}. \tag{24}$$

The momenta are given by

$$P_{j,1} = \tfrac{1}{2} m D x_j, \tag{25}$$

$$P_{j,2} = -\tfrac{1}{2} m x_j, \tag{26}$$

and the Hamiltonian by

$$H = \sum_{j=1}^{3} P_{j,1} D x_j + \sum_{j=1}^{3} P_{j,2} D^2 x_j + \tfrac{1}{2} \sum_{j=1}^{3} m x_j D^2 x_j + V(x_1, x_2, x_3), \tag{27}$$

which is equal to the energy.

Since we would expect the Hamiltonian to be a function of only pairs of canonical variables, we must replace the term involving $D^2 x_j$. Normally, the equations analogous to (25) and (26) would be used to eliminate the odd variable, usually the velocity. Obviously they can not be used here. If, rather, the equation of motion (24) is used, the Hamiltonian becomes

$$H = \sum_{j=1}^{3} P_{j,1} D x_j - \frac{1}{m} \sum_{j=1}^{3} P_{j,2} \frac{\partial V}{\partial x_j} - \tfrac{1}{2} \sum_{j=1}^{3} x_j \frac{\partial V}{\partial x_j} + V(x_1, x_2, x_3). \tag{28}$$

Let us symmetrically insert Eqs. (25) and (26) into the Hamiltonian

$$\begin{aligned} H = {} & \frac{1}{2}\left[\sum_{j=1}^{3} P_{j,1} D x_j + \sum_{j=1}^{3} P_{j,1} D x_j\right] \\ & - \frac{1}{2m}\left[\sum_{j=1}^{3} P_{j,2} \frac{\partial V(x_j)}{\partial x_j} + \sum_{j=1}^{3} P_{j,2} \frac{\partial V(x_j)}{\partial x_j}\right] \\ & - \frac{1}{4}\left[\sum_{j=1}^{3} x_j \frac{\partial V(x_j)}{\partial x_j} + \sum_{j=1}^{3} x_j \frac{\partial V(x_j)}{\partial x_j}\right] \\ & + \tfrac{1}{2}[V(x_j) + V(x_j)] \end{aligned} \tag{29}$$

$$\begin{aligned} = {} & \frac{1}{2}\left[\sum_{j=1}^{3} \frac{2P_{j,1}^2}{m} + \sum_{j=1}^{3} \frac{m(Dx_j)^2}{2}\right] \\ & - \frac{1}{2m}\left[-\sum_{j=1}^{3} \frac{m}{2} P_{j,2} \frac{\partial V(P_{j,2})}{\partial P_{j,2}} - \sum_{j=1}^{3} \frac{m x_j}{2} \frac{\partial V(x_j)}{\partial x_j}\right] \\ & - \frac{1}{4}\left[\sum_{j=1}^{3} P_{j,2} \frac{\partial V(P_{j,2})}{\partial P_{j,2}} + \sum_{j=1}^{3} x_j \frac{\partial V(x_j)}{\partial x_j}\right] \\ & + \tfrac{1}{2}[V(P_{j,2}) + V(x_j)] \end{aligned} \tag{30}$$

$$= \sum_{j=1}^{3} \frac{(P_{j,1})^2}{m} + \sum_{j=1}^{3} \frac{m}{4} (Dx_j)^2 + \tfrac{1}{2} V(P_{j,2}) + \tfrac{1}{2} V(x_j). \tag{31}$$

With the Hamiltonian in this form the canonical equations are

$$DP_{j,1} \equiv -\frac{\partial H}{\partial x_j} = -\frac{1}{2} \frac{\partial V(x_j)}{\partial x_j}, \tag{32}$$

$$DP_{j,2} \equiv -\frac{\partial H}{\partial D x_j} = -\frac{m}{2} D x_j, \tag{33}$$

$$D(x_j) \equiv \frac{\partial H}{\partial P_{j,1}} = \frac{2P_{j,1}}{m}, \tag{34}$$

$$D(Dx_j) \equiv \frac{\partial H}{\partial P_{j,2}} = \frac{1}{2} \frac{\partial V(P_{j,2})}{\partial P_{j,2}}. \tag{35}$$

If Eq. (19) is used for quantization, the wavefunction will depend on both x_j and Dx_j. From the

form of the Hamiltonian in Eq. (31) it appears that separation of variables may be assumed. Also, since both operators Dx_j and $P_{j,1}$ relate to the observable velocity, we must have

$$\langle Dx_j \rangle = \frac{2}{m}\left\langle C(1,2)\frac{\hbar}{i}\frac{\partial}{\partial x_j}\right\rangle. \tag{36}$$

This will be illustrated in Sec. V.

Regarding the correspondence with the uncertainty principle, it appears that since $P_{j,1}$ equals $mDx_j/2$ instead of mDx_j, we must set

$$C(1,2) = \tfrac{1}{2}. \tag{37}$$

Similarly, we must have

$$C(2,2) = \tfrac{1}{2}. \tag{38}$$

V. HARMONIC OSCILLATOR

The Lagrangian for a particle of mass m attached to a spring of spring constant k may be chosen as

$$L = -\frac{m}{2}xD^2x - \frac{k}{2}x^2, \tag{39}$$

whose equation of motion is

$$mD^2x = -kx. \tag{40}$$

Expressing the Hamiltonian in the form of Eq. (31) and using the quantization prescribed by Eqs. (19), (37), and (38), we have

$$\left[-\frac{\hbar^2}{4m}\frac{\partial^2}{\partial x^2} + \frac{m(Dx)^2}{4} - \frac{k\hbar^2}{4m^2}\frac{\partial^2}{\partial(Dx)^2} + \frac{kx^2}{4}\right]\Psi_n = E_n\Psi_n. \tag{41}$$

Assuming separation of variables

$$\Psi_n(x, Dx) = \Phi_n(x)\chi_n(Dx) \tag{42}$$

gives

$$-\frac{\hbar^2}{4m}\frac{d^2}{dx^2}\Phi_n + \frac{kx^2}{4}\Phi_n = C_n\Phi_n \tag{43}$$

and

$$\frac{k\hbar^2}{4m^2}\frac{d^2\chi_n}{d(Dx)^2} - \frac{m(Dx)^2}{4}\chi_n + E_n\chi_n = C_n\chi_n, \tag{44}$$

where C_n is the constant resulting from the separation.

Finite solutions for the powers series to Eq. (43) occur if there is some integer n for which

$$C_n = \tfrac{1}{4}\hbar\omega(2n+1). \tag{45}$$

Similarly, Eq. (44) will have a finite solution if

$$E_n - C_n = \tfrac{1}{4}\hbar\omega(2n+1). \tag{46}$$

Combining Eqs. (45) and (46) gives

$$E_n = (n + \tfrac{1}{2})\hbar\omega. \tag{47}$$

The wavefunction normalized to unity over the infinite range of x and Dx is

$$\Psi_n = \frac{1}{2^n n!}\left(\frac{m}{\pi\hbar}\right)^{\frac{1}{2}} H_n\left[\left(\frac{km}{\hbar^2}\right)^{\frac{1}{4}}x\right] H_n\left[\left(\frac{m^3}{k\hbar^2}\right)^{\frac{1}{4}}Dx\right] \times \exp\left[\frac{-m(Dx)^2 - kx^2}{2\hbar\omega}\right], \tag{48}$$

where $H_n(Y)$ is the Hermite polynomial.

If the expectation is calculated,

$$0 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Psi_n^* 0 \Psi_n \, dx \, d(Dx), \tag{49}$$

one finds

$$\langle x\rangle = \langle Dx\rangle = \langle P_1\rangle = \langle P_2\rangle = 0, \tag{50}$$

as is required, and

$$\left\langle \frac{2}{m}P_1^2\right\rangle = \left\langle \frac{m}{2}(Dx)^2\right\rangle = \left\langle \frac{k}{2}x^2\right\rangle = \left\langle \frac{2k}{m^2}P_2^2\right\rangle = \frac{\hbar\omega}{4}, \tag{51}$$

as is required for the ground state.

Similarly, a combination of Eqs. (19) and (20) can be used to give the wavefunction in $x \cdot P_2$, $Dx \cdot P_1$, or $P_1 \cdot P_2$ spaces. In each case we must take $C(1,2)$ and $C(2,2)$ to be $\frac{1}{2}$ to obtain results consistent with what is known to be the energy eigenvalues and expectation values for the harmonic oscillator.

VI. CONCLUSION

We have shown that it is possible to replace the usual Lagrangian containing derivatives of only first order by one with second-order derivatives and that such a change leaves the equations of motion intact and the Hamiltonian still equivalent to the energy. However, there is a change in the definition of the generalized momenta which results in a different form for the uncertainty principle and the rules for quantization. The resulting wavefunction has a mixed representation, but gives the usual energy eigenvalues and expectation values.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Rigorous Results for Ising Ferromagnets of Arbitrary Spin*

ROBERT B. GRIFFITHS†
Department of Physics, Carnegie-Mellon University, Pittsburgh, Pennsylvania

(Received 5 August 1968)

The following results for spin-$\frac{1}{2}$ Ising ferromagnets are extended to the case of arbitrary spin: (1) the theorem of Lee and Yang, that the zeros of the partition function lie on the unit circle in the complex fugacity plane; (2) inequalities of the form $\langle AB\rangle \geq \langle A\rangle\langle B\rangle$, where A and B are products of spin operators; (3) the existence of spontaneous magnetization on suitable lattices. Results (2) and (3) are also extended to the infinite-spin limit in which the spin variable is continuous on the interval $-1 \leq x \leq 1$.

1. INTRODUCTION

The standard Ising model which has been extensively studied in the theory of magnetic systems, alloys, fluid phase transitions, etc., is a "spin-$\frac{1}{2}$" model in the sense that the "spin variable" σ_i associated with a particular particle or lattice site can take on only the values $+1$ and -1, corresponding to the two eigenvalues of the z component of angular momentum for a particle of spin $\frac{1}{2}\hbar$. A natural extension of this model is one in which the spin variable may take on the $p+1$ values $p, p-2, p-4, \cdots, 2-p, -p$, corresponding to eigenvalues of the z component of angular momentum for a particle of spin $p/2$ (times $\hbar$). This generalization of the Ising model has been considered occasionally in the literature,[1] though it has received much less attention than the spin-$\frac{1}{2}$ case. Upon dividing the spin variable by p and taking the limit $p \to \infty$, one obtains the "infinite spin" or "classical Ising" model,[2] one of a variety of lattice systems with continuous variables (others include the spherical model and the "classical Heisenberg" model) which are of some interest in the statistical mechanics of phase transitions.

Our purpose in this paper is to extend to the case of arbitrary spin greater than $\frac{1}{2}$ certain results which are known to be true under very general conditions for spin-$\frac{1}{2}$ Ising systems with entirely ferromagnetic exchange interactions: (1) the inequalities of Kelly and Sherman[3] (which generalize some earlier results by the author[4]) of the form $\langle AB\rangle \geq \langle A\rangle\langle B\rangle$, where A and B represent products of spin variables; (2) the theorem of Lee and Yang,[5] which states that zeros of the partition function lie on the unit circle in the complex fugacity plane[6]; (3) proofs of the existence of phase transitions in two-, three-, and higher-dimensional lattices. Results (1) and (3) will also be extended to the infinite-spin (classical) Ising model, thereby showing, for example, that this model with nearest-neighbor ferromagnetic interactions on a square or simple cubic lattice undergoes a phase transition.

In each case, the extension is carried out by means of a representation of an Ising particle of spin $p/2$ in terms of a cluster of p spin-$\frac{1}{2}$ particles interacting among themselves through suitable ferromagnetic pair interactions. The idea of the representation is explained in Sec. 2, while Sec. 3 shows how to construct appropriate ferromagnetic representations for arbitrary spin. Once these representations are in hand, the extensions (1) to (3) mentioned above are quite straightforward and the details will be found in Sec. 4.

2. REPRESENTATION IN TERMS OF SPIN-$\frac{1}{2}$ PARTICLES

Consider an Ising "particle" of spin $p/2$, for which the variable S takes on the values $p, p-2, p-4, \cdots, -p$. We shall write S as a sum

$$S = \sigma_1 + \sigma_2 + \cdots + \sigma_p, \tag{2.1}$$

where the σ_i are "ordinary" Ising variables which take on the values $+1$ and -1. Collectively they form a "cluster" which "represents" the variable S. Provided the *weight function* $W_p(\sigma_1, \cdots, \sigma_p)$ is properly chosen, we may write

$$\sum_S f(S) = \sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_p} W_p f(\sigma_1 + \sigma_2 + \cdots + \sigma_p) \tag{2.2}$$

for any function f. In (2.2) (and hereafter) we use the convention that, in summing over a variable where the limits are not specified, the variable takes on all (and nothing but) its allowed values. Thus the sum over S

* Research supported in part by the National Science Foundation.
† Alfred P. Sloan Research Fellow.
[1] C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) A240, 214 (1957); Phys. Rev. 128, 168 (1962); G. Horwitz and H. B. Callen, Phys. Rev. 124, 1757 (1961); M. Suzuki, B. Tsujiyama, and S. Katsura, J. Math. Phys. 8, 124 (1967); J. Ashkin and E. Teller, Phys. Rev. 64, 178 (1943); R. B. Potts, Proc. Cambridge Phil. Soc. 48, 106 (1952); D. D. Betts, Can. J. Phys. 42, 1564 (1964); H. W. Capel, Physica 32, 966 (1966); 33, 295 (1967); Phys. Letters 23, 327 (1966); R. B. Griffiths, Physica 33, 689 (1967).
[2] This model has been examined for a one-dimensional chain by G. S. Joyce, Phys. Rev. Letters 19, 581 (1967); C. J. Thompson, J. Math. Phys. 9, 241 (1968).
[3] D. G. Kelly and S. Sherman, J. Math. Phys. 9, 466 (1968).
[4] R. B. Griffiths, J. Math. Phys. 8, 478, 484 (1967).
[5] T. D. Lee and C. N. Yang, Phys. Rev. 87, 410 (1952).
[6] The result of Lee and Yang has recently been extended to Ising ferromagnets with spin 1 and $\frac{3}{2}$ by M. Suzuki [J. Math. Phys. 9, 2064 (1968)] and T. Asano [Progr. Theoret. Phys. (Kyoto) 40, 1328 (1968)].

is from $-p$ to p in steps of 2, while for σ_j it is over the two values ± 1 only.

We shall require that the weight function W_p be nonnegative, and it must obviously have the property that, for any q in the range $-p \leq q \leq p$ which differs from p by zero or an even integer,

$$\sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma} W_p(\sigma_1, \sigma_2 \cdots \sigma_p)\delta\left(\sum_{j=1}^{p}\sigma_j; q\right) = 1, \quad (2.3)$$

where

$$\begin{aligned} \delta(a; b) &= 1, \quad \text{if } a = b, \\ &= 0, \quad \text{if } a \neq b. \end{aligned} \quad (2.4)$$

As an example, consider the spin-1 case, $p = 2$. An obvious choice for W_2 is

$$\begin{aligned} W_2(1, 1) &= W_2(-1, -1) = 1, \\ W_2(1, -1) &= W_2(-1, 1) = \tfrac{1}{2}. \end{aligned} \quad (2.5)$$

We shall call W_p a *ferromagnetic pair* weight function provided it can be written in the form

$$\begin{aligned} W_p(\sigma_1, \sigma_2 \cdots \sigma_p) &= \prod_{i<j} [\tfrac{1}{2}(1 + \sigma_i\sigma_j) + \tfrac{1}{2}(1 - \sigma_i\sigma_j)X_{ij}] \\ &= \exp\left[\sum_{i<j} K_{ij}(\sigma_i\sigma_j - 1)\right], \end{aligned} \quad (2.6)$$

with

$$0 \leq X_{ij} = \exp -2K_{ij} \leq 1 \quad (2.7a)$$

or

$$0 \leq K_{ij} \leq \infty. \quad (2.7b)$$

While (2.6) looks complicated, it is really very simple: W_p, for a particular choice of $\sigma_1, \cdots, \sigma_p$, is a product of factors X_{ij}, one for each *pair* (ij) of spins for which $\sigma_i \neq \sigma_j$. The condition (2.7) corresponds to the requirement of *ferromagnetic* exchange within the cluster (see discussion below). We permit K_{ij} to have the value $+\infty$ (so that $X_{ij} = 0$); this case is not particularly pathological and turns out to be very useful. The example (2.5) is a ferromagnetic pair weight function with $X_{12} = \frac{1}{2}$ or $K_{12} = \frac{1}{2}\ln 2$.

A graphical representation of spin clusters with ferromagnetic pair weight functions proves useful for purposes of exposition and intuition; we shall not employ it formally in proofs. A particle of spin $\frac{1}{2}$ is represented by an open circle, and if $0 < X_{ij} < 1$, a line (or "bond") is drawn from i to j. If $X_{ij} = 0$, the circles representing i and j touch, whereas the line is absent if $X_{ij} = 1$. Figure 1 shows possible ferromagnetic pair representations for $p = 2$ [see (2.5)] and $p = 3$.

Consider a system (hereafter known as the "original system") of n Ising particles with spin variables S_1, $S_2, \cdots, S_n$. For the jth particle, S_j may take on the values $p_j, p_j - 2, \cdots, -p_j$, where p_j is a positive integer which may depend on j. The system has a Hamiltonian $H(S_1, \cdots, S_n)$, a real-valued function of the spin variables. The value $+\infty$ is permitted, but not $-\infty$, and for at least one choice of the variables H must be noninfinite [This insures that the partition function, Eq. (2.11), is nonzero].

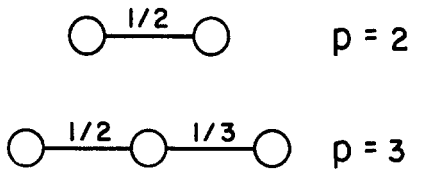


FIG. 1. Examples of ferromagnetic pair weight functions. Values of X_{ij} are noted next to line joining spins i and j.

We shall represent the variables S_j in terms of clusters of spin $\frac{1}{2}$:

$$S_j = \sum_{k=1}^{p_j}\sigma_{jk}, \quad (2.8)$$

where the σ_{ij} can take on the values ± 1. Let $W_j(\sigma_{j1}, \sigma_{j2}, \cdots)$ be a suitable weight function, i.e., nonnegative and satisfying (2.3) for $p = p_j$. By means of (2.8), any function $F(S_1, \cdots, S_n)$ (including the Hamiltonian H) may be expressed as a function of the σ_{ij}; since no confusion is likely to result, we shall use the same symbol for the function with either set of variables.

The collection of all the σ_{ij} will be known as the "analog" system and for this system we define the analog Hamiltonian $\hat{H}$ as

$$\begin{aligned} \hat{H}(\sigma_{11}\cdots) = H(S_1(\sigma_{11}\cdots)\cdots) \\ - \beta^{-1}\sum_{j=1}^{n}\ln W_j(\sigma_{j1}\cdots), \end{aligned} \quad (2.9)$$

where $\beta = (kT)^{-1}$ is the inverse temperature and we shall suppose that $0 < \beta < \infty$. (Note that the analog Hamiltonian is temperature dependent, a fact which is of no consequence for the purposes of this paper, but could be important in considering specific examples.)

If $F(S_1 \cdots S_n)$ is a function everywhere finite, we have

$$\begin{aligned} \mathrm{Tr}\,[Fe^{-\beta H}] &= \sum_{S_1}\cdots\sum_{S_n} Fe^{-\beta H} \\ &= \sum_{\sigma_{11}}\sum_{\sigma_{12}}\cdots\sum_{\sigma_{21}}\cdots\sum_{\sigma_{np_n}} W_1W_2\cdots W_nFe^{-\beta H} \\ &= \sum_{\sigma_{11}}\cdots\sum_{\sigma_{np_n}} Fe^{-\beta\hat{H}} \\ &= \hat{\mathrm{Tr}}\,[Fe^{-\beta\hat{H}}]. \end{aligned} \quad (2.10)$$

The symbol Tr (trace) is, in the present context, merely an abbreviation for the multiple summation. If $F = 1$,

(2.10) states that the partition functions

$$Z = \mathrm{Tr}\,[e^{-\beta H}] = \hat{\mathrm{Tr}}\,[e^{-\beta \hat{H}}] = \hat{Z} \qquad (2.11)$$

for the original and analog systems, respectively, are identical and (2.10) together with (2.11) implies that the thermal average of F,

$$\langle F \rangle = \mathrm{Tr}\,[Fe^{-\beta H}]/Z = \hat{\mathrm{Tr}}\,[Fe^{-\beta \hat{H}}]/\hat{Z}, \qquad (2.12)$$

is the same in both cases. Equations (2.11) and (2.12) are the basis of the extensions of the Lee–Yang theorem, etc. (see Sec. 4), but first we shall construct appropriate weight functions.

3. FERROMAGNETIC WEIGHT FUNCTIONS

Not only do there exist ferromagnetic weight functions for arbitrary spin $p/2$, but for $p \geq 3$ the choice is not unique. We shall explicitly construct a set of weight functions which are reasonably simple and at the same time of a form which proves useful when considering phase transitions (Sec. 4D).

Consider first the case where $p = 2r$ is an even integer. For notational convenience, separate the p σ's into two groups of r each, the first labeled by negative subscripts, $\sigma_{-1}, \sigma_{-2}, \cdots, \sigma_{-r}$, and the second with positive: $\sigma_1, \sigma_2, \cdots, \sigma_r$. All X_{ij} in (2.6) shall be set equal to 1, except for the following:

$$X_{-i,-i+1} = 0, \qquad \text{for } 2 \leq i \leq r, \qquad (3.1a)$$

$$X_{-1,1} = \tfrac{1}{2}, \qquad (3.1b)$$

$$X_{i,i+1} = 2/(2i+1), \qquad \text{for } 1 \leq i \leq r-1. \qquad (3.1c)$$

In particular, for $p = 2$, $X_{-1,1} = \frac{1}{2}$, while, for $p = 4$, $X_{-2,-1} = 0$, $X_{-1,1} = \frac{1}{2}$, $X_{1,2} = \frac{2}{3}$. (For graphical representations when $p = 2$, 4, and 6, see Figs. 1 and 2.)

The X_{ij} in (3.1) clearly satisfy (2.7). In addition, we must check (2.3). This need be done only for $q \geq 0$, since W_p is unchanged if $\sigma_i \to -\sigma_i$ for every i. An explicit calculation can be carried out for $p = 2$ and 4. For the latter, $W_4(\sigma_{-2}, \sigma_{-1}, \sigma_1, \sigma_2)$ is nonvanishing in the following cases:

$$q = 4\text{: } W(1,1,1,1) = 1,$$

$$q = 2\text{: } W(1,1,1,-1) = \tfrac{2}{3}, \quad W(1,1,-1,1) = \tfrac{1}{3},$$

$$q = 0\text{: } W(1,1,-1,-1) = \tfrac{1}{2},$$

$$W(-1,-1,1,1) = \tfrac{1}{2}. \qquad (3.2)$$

The condition (3.1a) serves to "lock together" all the σ's with negative subscripts, so that if W_p is not to vanish, one of two possibilities

$$\sigma_{-r} = \sigma_{-r+1} = \cdots = \sigma_{-1} = 1, \qquad (3.3a)$$

$$\sigma_{-r} = \sigma_{-r+1} = \cdots = \sigma_{-1} = -1 \qquad (3.3b)$$

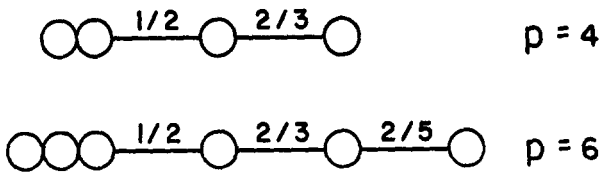


FIG. 2. Weight functions for p even.

must occur. For $q = 0$, there are precisely two nonvanishing terms in (2.3): (3.3a) together with $\sigma_1 = \sigma_2 = \cdots = \sigma_r = -1$, and (3.3b) together with $\sigma_1 = \sigma_2 = \cdots = 1$; in either case $W_p = X_{-1,1} = \frac{1}{2}$ and (2.3) is satisfied.

For $q > 0$, all the nonvanishing terms in (2.3) correspond to (3.3a). We shall divide the sum in (2.3) into two parts:

$$U_p(q) = \sum_{\sigma_1} \cdots \sum_{\sigma_{r-1}} W_p(1, \cdots, 1, \sigma_1, \cdots, \sigma_{r-1}, 1) \times \delta\left(\sum_j \sigma_j; q\right), \qquad (3.4)$$

$$V_p(q) = \sum_{\sigma_1} \cdots \sum_{\sigma_{r-1}} W_p(1, \cdots, 1, \sigma_1, \cdots, \sigma_{r-1}, -1) \times \delta\left(\sum_j \sigma_j; q\right). \qquad (3.5)$$

These definitions yield immediately the special values

$$U_p(0) = 0, \quad V_p(p) = 0. \qquad (3.6)$$

The result

$$W_{p+2}(1, \cdots, 1, \sigma_1, \cdots, \sigma_r, \sigma_{r+1}) = W_p(1, \cdots, 1, \sigma_1, \cdots, \sigma_r)\delta(\sigma_r; \sigma_{r+1}) + [2/(p+1)]W_p(1, \cdots, 1, \sigma_1, \cdots, \sigma_r)\delta(\sigma_r; -\sigma_{r+1}) \qquad (3.7)$$

(note that the first $r+1$ arguments of W_{p+2}, but only the first r arguments of W_p, are always equal to 1) is a consequence of (3.1) and provides the following recursion relations for U and V, for q (which is an even integer) in the range $0 \leq q \leq p$:

$$U_{p+2}(q+2) = U_p(q) + \frac{2}{p+1} V_p(q), \qquad (3.8a)$$

$$V_{p+2}(q) = V_p(q) + \frac{2}{p+1} U_p(q). \qquad (3.8b)$$

The expressions

$$U_p(q) = (q-1)/(p-1), \quad \text{for } 0 < q \leq p, \quad = 0, \quad \text{for } q = 0, \qquad (3.9a)$$

$$V_p(q) = (p-q)/(p-1), \quad \text{for } 0 < q \leq p, \quad = \tfrac{1}{2}, \quad \text{for } q = 0, \qquad (3.9b)$$

satisfy the recursion relations (3.8), agree with the special values (3.6), and for $p = 4$ coincide with (3.2). (They are also correct for $p = 2$.) Hence, they are

correct for general q and p. Since, further, $U_p(q) + V_p(q) = 1$ for $q > 0$, we have completed the proof that (3.1) inserted in (2.6) yields W_p, satisfying (2.3).

Next suppose that $p = r + t$ is odd, where $r = \frac{1}{2}(p+1)$ and $t = \frac{1}{2}(p-1)$. Separate the σ's into two groups, the first with negative subscripts, $\sigma_{-1}, \sigma_{-2}, \cdots, \sigma_{-r}$, and the second with positive, $\sigma_1, \sigma_2, \cdots, \sigma_t$. Let the first group be "locked together":

$$X_{-i,-i+1} = 0, \quad \text{for } 2 \leq i \leq r; \tag{3.10}$$

and for the second group choose X_{ij}, with i and j positive, so that $W_t(\sigma_1, \sigma_2, \cdots, \sigma_t)$, defined by (2.6) (with p replaced by t) is itself a ferromagnetic pair weight function. The X_{ij} not defined by these two conditions, in particular, those for which i is negative and j is positive shall be equal to 1. We must now check that W_p thus defined satisfies (2.3) for q an odd integer in the range $0 < q < p$.

Once again, if W_p is not to vanish, (3.3a) and (3.3b) represent the only possibilities for σ's in the first group and for $q > 0$ we must choose (3.3a). In addition we have

$$W_p(1, 1, \cdots, 1, \sigma_1, \sigma_2, \cdots, \sigma_t) = W_t(\sigma_1, \sigma_2, \cdots, \sigma_t) \tag{3.11}$$

and thus

$$\sum_{\sigma_{-r}} \cdots \sum_{\sigma_t} W_p(\sigma_{-r}, \cdots, \sigma_t)\delta\left(\sum_{j=-r}^{-1}\sigma_j + \sum_{j=1}^{t}\sigma_j; q\right) = \sum_{\sigma_1} \cdots \sum_{\sigma_t} W_t(\sigma_1, \cdots, \sigma_t)\delta\left(\sum_{j=1}^{t}\sigma_j; q - r\right) = 1. \tag{3.12}$$

The only remaining problem is to choose W_t for $t = \frac{1}{2}(p-1)$. There are several possibilities: for t even we may use (3.1), while for t odd we may apply the above construction once again, or we may simply employ (3.13) below for t even or odd. Figure 3 shows possible clusters for $p = 3$, 5, and 7.

As we stated earlier, the choice for ferromagnetic weight functions for $p \geq 3$ is not unique. The above choices will prove useful in Sec. 4D, but we here present still another which is somewhat simpler to construct, which works for both even and odd p, and for which none of the X_{ij} vanish. Namely, let all the X_{ij} $(1 \leq i < j \leq p)$ be 1 except for

$$X_{i,i+1} = 1/(i+1), \quad i = 1, 2, \cdots, p-1. \tag{3.13}$$

The cases $p = 2$ and 3 are illustrated in Fig. 1. We leave to the reader the proof that (2.3) is satisfied.

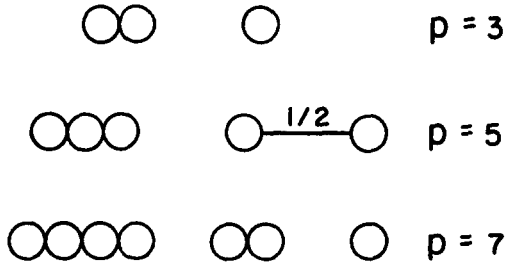


FIG. 3. Weight functions for p odd.

4. APPLICATIONS

A. Notation

As in Sec. 2, we consider a system of n Ising particles and represent the spin variable for the jth particle, S_j, in the form (2.8). For brevity, we shall occasionally relabel the σ_{jk} of the analog system as σ_α, where α runs from 1 to

$$m = \sum_{j=1}^{n} p_j. \tag{4.1}$$

A *multiplicity function* $\mu(i)$ assigns a nonnegative integer to each integer i in the range between 1 and n. Define

$$\phi(\mu) = \sum_{i=1}^{n} \mu(i), \tag{4.2}$$

$$S^\mu = \prod_{i=1}^{n} (S_i)^{\mu(i)}, \tag{4.3a}$$

$$P^\mu = \prod_{i=1}^{n} (p_i)^{\mu(i)}, \tag{4.3b}$$

with $(S^i)^0 = 1$. The Hamiltonian[7]

$$H = -\sum_{\mu} J_\mu (S^\mu - P^\mu) + \text{const} \tag{4.4}$$

will be called *ferromagnetic* provided

$$0 \leq J_\mu \leq \infty \tag{4.5}$$

for all multiplicity functions μ. We permit J_μ to take the value $+\infty$, in which case H is the limit (finite or infinite) of (4.4) as $J_\mu \to \infty$. [$S^\mu - P^\mu$ appears in (4.4) rather than S^μ to allow for the possibility of infinite J_μ; otherwise, the P^μ could be absorbed into the constant.] Note also that the sum in (4.4) may involve an infinite number of multiplicity functions.[8]

A special case of (4.4) is

$$H = -\sum_{i \leq j} J_{ij}(S_i S_j - p_i p_j) - \mathcal{H}\sum_i (S_i - p_i) + \text{const}, \tag{4.6}$$

[7] All Hamiltonians in this paper are understood to be defined only up to an additive (finite) constant, which is sometimes [as in (4.6)], but not always, explicitly noted.

[8] In principle, one can always rewrite (4.4) using only a finite number of multiplicity functions, since S^{p+1} may always be re-expressed as a linear combination of S to lower powers (including S^0). However, it is possible for (4.5) to be satisfied by the original Hamiltonian but not by the re-expressed version.

where J_μ vanishes whenever $\phi(\mu) > 2$ and $\mathcal{H}$ is the magnetic field.

B. The Inequality of Kelly and Sherman

Theorem 1: Let ν and λ be multiplicity functions, and let the J_μ for the Hamiltonian (4.4) satisfy (4.5). Then

$$\langle S^{\nu+\lambda}\rangle = \langle S^\nu S^\lambda\rangle \geq \langle S^\nu\rangle\langle S^\lambda\rangle. \tag{4.7}$$

Proof: Let $a, b, \cdots, d$ be a collection of $\phi(\nu)$ numbers drawn from the set $\{1, 2, \cdots, n\}$ in some arbitrary order but with the property that j occurs in the collection $\nu(j)$ times. Using (4.3) and (2.8), we have

$$\begin{aligned} S^\nu &= \left(\sum_i \sigma_{ai}\right)\left(\sum_j \sigma_{bj}\right)\cdots\left(\sum_k \sigma_{dk}\right) \\ &= \sum_i\sum_j\cdots\sum_k \sigma_{ai}\sigma_{bj}\cdots\sigma_{dk}, \end{aligned} \tag{4.8}$$

where i ranges from 1 to p_a, etc.

Since $(\sigma_{jk})^2 = 1$, it is possible to replace a term like $(\sigma_{jk})^l$ appearing in one of the summands of (4.8) by 1 if l is even and σ_{jk} if l is odd. Thus it is clear that (4.4) expressed as a function of the σ_α has the form used by Kelly and Sherman,[3] as does the analog Hamiltonian[7] (2.9):

$$\hat{H} = -\sum_A \hat{J}_A(\sigma^A - 1), \tag{4.9}$$

where the A's are subsets of $M = \{1, 2, \cdots, m\}$, and

$$\sigma^A = \prod_{\alpha\in M}\sigma_\alpha. \tag{4.10}$$

Further, since the J_μ satisfy (4.5) and we employ ferromagnetic pair weight functions satisfying (2.7), it is clear that

$$0 \leq \hat{J}_A \leq \infty. \tag{4.11}$$

Finally, to verify (4.7), we only need to write it out in terms of the σ's. Let $a', b', \cdots, d'$ be a collection of $\phi(\lambda)$ numbers taken from $\{1, 2, \cdots, n\}$ in such a way that j occurs in the collection $\lambda(j)$ times. Then

$$\begin{aligned} &\langle S^\nu S^\lambda\rangle \\ &= \left\langle \sum_i\sum_j\cdots\sum_k\sum_{i'}\sum_{j'}\cdots\sum_{k'} \sigma_{ai}\sigma_{bj}\cdots\sigma_{dk}\sigma_{a'i'}\sigma_{b'j'}\cdots\sigma_{d'k'}\right\rangle \\ &= \sum_i\sum_j\cdots\sum_k\sum_{i'}\sum_{j'}\cdots\sum_{k'}\langle\sigma_{ai}\sigma_{bj}\cdots\sigma_{dk}\sigma_{a'i'}\sigma_{b'j'}\cdots\sigma_{d'k'}\rangle \\ &\geq \sum_i\sum_j\cdots\sum_k\sum_{i'}\sum_{j'}\cdots\sum_{k'}\langle\sigma_{ai}\sigma_{bj}\cdots\sigma_{dk}\rangle\langle\sigma_{a'i'}\sigma_{b'j'}\cdots\sigma_{d'k'}\rangle \\ &= \left\langle\sum_i\sum_j\cdots\sum_k \sigma_{ai}\sigma_{bj}\cdots\sigma_{dk}\right\rangle \\ &\quad\times\left\langle\sum_{i'}\sum_{j'}\cdots\sum_{k'}\sigma_{a'i'}\sigma_{b'j'}\cdots\sigma_{d'k'}\right\rangle \\ &= \langle S^\nu\rangle\langle S^\lambda\rangle, \end{aligned} \tag{4.12}$$

where we have used the inequality of Kelly and Sherman, which is (4.7) for the case $p_i = 1$ for all i (spin-$\frac{1}{2}$ particles), in order to obtain the inequality in (4.12).

Note that the possibility of infinite values for H—either because some of the J_μ are infinite, or because of summing over an infinite number of finite J_μ—causes no difficulty. In particular, H is always noninfinite if $S_j = p_j$ for all j, and thus Z in (2.11) and (2.12) does not vanish.

C. Theorem of Lee and Yang on Zeros of the Partition Function

Theorem 2: If the J_{ij} in the Hamiltonian (4.6) satisfy (4.5), the zeros of the partition function (2.11), a polynomial in the variable

$$z = e^{-2\beta\mathcal{H}}, \tag{4.13}$$

lie on the unit circle $|z| = 1$ in the complex z plane.

Proof: With the help of a ferromagnetic pair weight function, the analog Hamiltonian corresponding to (4.6) may be expressed in the form[7]

$$\hat{H} = -\sum_{\alpha<\beta}\hat{J}_{\alpha\beta}(\sigma_\alpha\sigma_\beta - 1) - \mathcal{H}\sum_\alpha(\sigma_\alpha - 1), \tag{4.14}$$

with the $\hat{J}_{\alpha\beta}$ in the range $[0, \infty]$. Lee and Yang[5] have shown that under these circumstances the zeros of the analog partition function regarded as a function of z lie on the circle $|z| = 1$. But, of course, the original and analog systems have identical partition functions (2.11).

D. Phase Transitions

Assume that $p_i = p$ is the same for all Ising particles and define the normalized spin variables

$$s_i = S_i/p. \tag{4.15}$$

Let the Hamiltonian[7] be

$$H = -r_1\sum_{i\leq j}J_{ij}(s_is_j - 1) - r_2\sum_i\mathcal{H}_is_i, \tag{4.16}$$

where the scaling factors r_1 and r_2 are always assumed to be positive. We shall employ the special weight functions defined by (3.1) and (3.10), and in place of (2.8) write

$$s_j = u_j + v_j = p^{-1}\sum_{k<0}\sigma_{jk} + p^{-1}\sum_{k>0}\sigma_{jk}, \tag{4.17}$$

that is, u_j represents the spins in the cluster which are "locked together" by the weight functions. It can take on the values $\pm q$, where $q = \frac{1}{2}$ or $(p+1)/2p$ for p even or odd, respectively.

Let

$$M_p(r_1, r_2) = \langle s_l\rangle = \langle u_l\rangle + \langle v_l\rangle \tag{4.18}$$

be the "magnetization" of a particular particle l.

Theorem 3: Provided the J_{ij} and $\mathcal{H}_i$ in (4.16) are all nonnegative,

$$\tfrac{1}{2}M_1(r_1/4, r_2/2) \leq M_p(r_1, r_2) \leq M_1(r_1, r_2), \quad (4.19)$$

where M_1 is the value of $\langle s_l \rangle$ in the case $p = 1$ (spin-$\frac{1}{2}$ particles).

Proof: We shall make essential use of the fact that in the analog system the $\langle \sigma_\alpha \rangle$ are all nonnegative and monotone nondecreasing functions of the $\hat{J}_A$ in (4.9), provided these are all nonnegative—a consequence of the inequality (4.7), and worked out for the restricted class of Hamiltonian considered here in Ref. 4. These $\hat{J}_A$ include both terms arising from the J_{ij} and $\mathcal{H}_i$ in (4.16) and also the K_{ij}[9] which appear in the weight functions (2.6). Thus, if the K_{ij} are increased to infinity in each cluster, $\langle s_l \rangle$ cannot decrease. But this locks together all the spins in a cluster, so that s_i can only take the values ± 1, and (4.16) becomes the Hamiltonian for a system of spin-$\frac{1}{2}$ particles ($p = 1$). This establishes the second inequality in (4.19).

To establish the first inequality, insert (4.17) in (4.16) and use (2.9) to obtain the analog Hamiltonian[7]:

$$\begin{aligned}\hat{H} = &-r_1 \sum_{i \leq j} J_{ij}(u_i u_j - q^2) - r_2 \sum_i \mathcal{H}_i u_i \\ &- \Big\{ r_1 \sum_{i \leq j} J_{ij}[u_i v_j + u_j v_i + v_i v_j + q^2 - 1] \\ &+ r_2 \sum_i \mathcal{H}_i v_i \Big\} - \beta^{-1} \sum_j \ln W_j. \end{aligned} \quad (4.20)$$

Define a new Hamiltonian $\hat{H}'$ by replacing by zero all terms in curly brackets in (4.20) and also all K_{ij} in the weight functions *except* those which lock together the spins in each u_k. Since u_k can only take the values $\pm q$, let us write

$$u_k = q\bar{\sigma}_k \quad (4.21)$$

and

$$\hat{H}' = -r_1 q^2 \sum_{i \leq j} J_{ij}(\bar{\sigma}_k \bar{\sigma}_j - 1) - r_2 q \sum_i \mathcal{H}_i \bar{\sigma}_i. \quad (4.22)$$

Since $\hat{H}'$ is obtained from $\hat{H}$ by reducing various of the $\hat{J}_A$ to zero, it is clear that $\langle u_l \rangle'$ in the new system is a lower bound for $\langle u_l \rangle$ in the original system, which is, in turn, a lower bound for M_p. However, (4.22) is identical with (4.16) when $p = 1$, apart from changes in the scaling factors. These two observations, together with $q \geq \frac{1}{2}$, establish the first inequality in (4.19).

If $r_2 = 0$, M_p always vanishes because (4.16) is then unchanged if all the s_i are replaced by $-s_i$. However, if one evaluates $M_p = \langle s_l \rangle$ in the limit of an infinite system with $r_2 > 0$ and then takes the limit $r_2 \to 0$, it may happen that M_p in this limit is positive (we assume $\mathcal{H}_i \geq 0$). If this is the case, the system is said to exhibit a "spontaneous magnetization."[10] There are a number of cases where Ising ferromagnets of spin-$\frac{1}{2}$ are known to exhibit a spontaneous magnetization at temperatures $T < T_c(1)$, the Curie temperature, and no spontaneous magnetization at higher temperatures.[11] In these cases, (4.19) implies that the corresponding spin-$p/2$ ferromagnet has a Curie temperature $T_c(p)$ in the range

$$\tfrac{1}{4}T_c(1) \leq T_c(p) \leq T_c(1), \quad (4.23)$$

provided the values of J_{ij} are the same in both cases, with the normalization used in (4.16).

E. The Infinite-Spin (Classical) Limit

The continuous variables x_i for a system of n "infinite-spin" or "classical" Ising particles take on values in the range $-1 \leq x_i \leq 1$. We shall assume a Hamiltonian

$$H^* = -\sum_\mu J_\mu x^\mu + \text{const}, \quad (4.24)$$

where the sum is over multiplicity functions, and x^μ is defined in analogy with S^μ in (4.3a). In the ferromagnetic case we require

$$0 \leq J_\mu < \infty \quad (4.25)$$

(infinite values are not permitted) and, if $J_\mu > 0$ for an infinite number of multiplicity functions, we shall further demand that

$$\sum_\mu J_\mu < \infty \quad (4.26)$$

to insure that the convergence of (4.24) is uniform. The partition function and the thermal average of a continuous function F are defined by

$$Z^* = \int_{-1}^{1} dx_1 \int_{-1}^{1} dx_2 \cdots \int_{-1}^{1} dx_n e^{-\beta H^*}, \quad (4.27)$$

$$\langle F \rangle^* = \int_{-1}^{1} dx_1 \cdots \int_{-1}^{1} dx_n F(x_1 \cdots x_n) e^{-\beta H^*}/Z^*. \quad (4.28)$$

We wish to regard the infinite-spin case as a limit of systems with finite spin. Consider n Ising particles

[9] Of course, as long as (2.3) is satisfied, M_p will be independent of the K_{ij}, but we have in mind variations of the latter which will alter the left side of (2.3).

[10] There are a number of subtleties involved in the definition of spontaneous magnetization; see the discussion in R. B. Griffiths, Phys. Rev. **152**, 240 (1966).

[11] In addition to the well-known case of nearest-neighbor interaction on a square lattice, for which the magnetization has been calculated by C. N. Yang [Phys. Rev. **85**, 808 (1952), but see the comments in T. D. Schultz, D. C. Mattis, and E. H. Lieb, Rev. Mod. Phys. **36**, 856 (1964), especially p. 870], rigorous results are also known for some three-dimensional lattices: C.-Y. Weng, R. B. Griffiths, and M. E. Fisher, Phys. Rev. **162**, 475 (1967); M. E. Fisher, Phys. Rev. **162**, 480 (1967); R. B. Griffiths, Commun. Math. Phys. **6**, 121 (1967).

of spin $p/2$ with variables s_i defined by (4.15) and s^μ in analogy with (4.3a). The Hamiltonian is

$$H_p = -\sum_\mu J_\mu s^\mu, \tag{4.29}$$

while the partition function Z_p and the thermal average $\langle F\rangle_p$ are defined as in (2.11) and (2.12).

Theorem 4: If the J_μ satisfy (4.25) and (4.26), then

$$\lim_{p\to\infty}\left(\frac{2}{p}\right)^n Z_p = Z^* > 0 \tag{4.30}$$

and, if F is a continuous function,

$$\lim_{p\to\infty}\langle F\rangle_p = \langle F\rangle^*. \tag{4.31}$$

The theorem is, of course, no more than the observation that Riemann integrals are the limits of approximating sums. Nonetheless, it is useful to write it down, since it has some interesting consequences:

Corollary 4.1: When conditions (4.25) and (4.26) are satisfied and ν and λ are multiplicity functions,

$$\langle x^{\nu+\lambda}\rangle = \langle x^\nu x^\lambda\rangle \geq \langle x^\nu\rangle\langle x^\lambda\rangle. \tag{4.32}$$

The result is obtained by combining Theorems 1 and 4.

Corollary 4.2: The bounds (4.19) and (4.23) also apply in the limit $p \to \infty$, with S_i replaced everywhere by x_i in (4.16), provided none of the J_{ij} are infinite.

The second corollary, in particular, is interesting, since it provides a proof that on a square or simple cubic lattice, the infinite-spin model with nearest-neighbor interactions exhibits a spontaneous magnetization at sufficiently low temperatures. This result, while it is not particularly surprising, has not (we believe) hitherto been proved in a rigorous fashion. It is possible that one might work out a direct proof in analogy with the Peierls argument[12] for the spin-$\frac{1}{2}$ case and gain additional insight into the mechanism of the phase transition, but thus far we have not succeeded.

5. CONCLUSION

One of the outstanding problems in statistical mechanics at the present time is the extent to which the many interesting results in the theory of phase transitions for the spin-$\frac{1}{2}$ Ising model are specific to this model and to what extent they have a more general application. We believe our results represent a very modest beginning in answering this question for the particular features of the Ising model with which we have been concerned. The representations of Ising particles with spin greater than $\frac{1}{2}$ in terms of those with spin $\frac{1}{2}$ seems to be a useful tool and may well have applications outside of those we have discussed.

ACKNOWLEDGMENTS

We would like to acknowledge the stimuli provided by discussions and correspondence with Professor S. Sherman and discussions with Mr. C.-Y. Weng.

[12] R. Peierls, Proc. Cambridge Phil. Soc. **32**, 477 (1936); R. B. Griffiths, Phys. Rev. **136**, A437 (1964); R. L. Dobrushin, Theory Probability Appl. (USSR) **10**, 193 (1965).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Conserved Quantities in the Einstein–Maxwell Theory*

ALBERT R. EXTON† AND EZRA T. NEWMAN
University of Pittsburgh, Pittsburgh, Pennsylvania
AND
ROGER PENROSE
Birkbeck College,‡ University of London, London, England

(Received 8 March 1967)

It is shown that the 10 gravitationally-conserved quantities defined in asymptotically flat, empty, space-times are, when suitably modified, also conserved in asymptotically flat Einstein–Maxwell space-times. Furthermore, the implied selection rules for transitions between stationary Einstein–Maxwell states are the same as those in the pure gravitational case.

I. INTRODUCTION

It has recently been shown[1,2] that in Einstein vacuum gravitational theory there are ten quantities, defined for asymptotically flat space-times, which are absolutely conserved. In the Einstein–Maxwell theory there are six conserved quantities which are the analogs of the above for the Maxwell field. In a stationary vacuum field, these ten conserved quantities can be expressed as certain combinations of the mass, dipole, and quadrupole moments. This fact leads to a selection rule for purely gravitational transitions between stationary states, namely, that if a field is initially stationary and then becomes radiative, if it is ever to become stationary again, the combination of moments mentioned above must return to its original value.

The purpose of this paper is to show that in asymptotically flat Einstein–Maxwell space-times there are 16 conserved quantities—the six mentioned in Refs. 1 and 2 and, in addition, ten which are closely related to the ten conserved quantities in the pure gravitational case. In stationary states, these ten quantities reduce to the same combination of moments as in the vacuum case. Thus, we have the same selection rules for transitions between stationary Einstein–Maxwell states as for vacuum states with additional selection rules arising from the six Maxwell conserved quantities.

II. ASYMPTOTIC BEHAVIOR

The conservation laws reported in Refs. 1 and 2 were arrived at by consideration of the asymptotic behavior of the fields in question. We shall, therefore, investigate the asymptotic behavior of the Einstein–Maxwell field using the method of Newman–Unti (N–U).[3] We adopt essentially[4] the same coordinate and tetrad conditions used there, where, of course, we use the field equations and Bianchi Identities appropriate to the Einstein–Maxwell field as given by Newman and Penrose.[5] Using the results of Kozarzewski[6] for the asymptotic behavior of the spin coefficients and the peeling-off property of the fields, one obtains by the method of N–U the following asymptotic form for the Einstein–Maxwell field. If

$$\psi_0 = \psi_0^0 \mathfrak{r}^{-5} + \psi_0^1 \mathfrak{r}^{-6} + O(\mathfrak{r}^{-7}), \tag{1}$$

$$\phi_0 = \phi_0^0 \mathfrak{r}^{-3} + \phi_0^1 \mathfrak{r}^{-4} + O(\mathfrak{r}^{-5}), \tag{2}$$

and the various $\mathfrak{u}$, θ, φ derivatives of these expressions also hold, then

$$\psi_1 = \psi_1^0 \mathfrak{r}^{-4} + (\bar{\delta}\psi_0^0 + 3\bar{\phi}_1^0\phi_0^0)\mathfrak{r}^{-5} + O(\mathfrak{r}^{-6}), \tag{3}$$

$$\psi_2 = \psi_2^0 \mathfrak{r}^{-3} + (\bar{\delta}\psi_1^0 + 2\phi_1^0\bar{\phi}_1^0)\mathfrak{r}^{-4} + O(\mathfrak{r}^{-5}), \tag{4}$$

* Work supported, in part, by the Aerospace Research Laboratories, Office of Aerospace Research, U.S. Air Force.

† Andrew Mellon Fellow. Present address: The University of Texas, Austin, Texas.

‡ This work was done while the author was at Yeshiva and Princeton Universities.

[1] E. Newman and R. Penrose, Phys. Rev. Letters **15**, 231 (1965).

[2] E. Newman and R. Penrose, Proc. Roy. Soc. (London) **305**, 175 (1968).

[3] E. Newman and T. Unti, J. Math. Phys. **3**, 891 (1962).

[4] Some slight changes in the notation from that of Refs. 3 and 8 are being introduced here (and in Ref. 2), although agreement with Ref. 7 is being maintained. This results in a somewhat simplified appearance of most of the equations; in particular, the removal of all factors of $(2)^{\frac{1}{2}}$. To emphasize that the notation has been altered from that of Refs. 3 and 8, the retarded time and radial coordinates, respectively, are being denoted here by $\mathfrak{u}$ and $\mathfrak{r}$, with lower case ψ's for the Weyl tensor components. Indicating by primed letters those quantities defined in Refs. 3, 8, the translation to the present notation is achieved by

$$u' = 2^{\frac{1}{2}}\mathfrak{u}, \quad r' = 2^{-\frac{1}{2}}\mathfrak{r}, \quad l^{\mu'} = 2^{\frac{1}{2}}l^{\mu}, \quad m^{\mu'} = m^{\mu}, \quad n^{\mu'} = 2^{-\frac{1}{2}}n^{\mu};$$

thus, we have

$$\Psi_n' = 2^{\frac{1}{2}(2-n)}\psi_n, \quad \Psi_n^{m'} = 2^{-\frac{1}{2}(3-m)}\psi_n^m, \quad \dot{\Psi}_n^{m'} = 2^{-\frac{1}{2}(4+m)}\dot{\psi}_n^m,$$

$$\Phi_n' = 2^{\frac{1}{2}(1-n)}\phi_n, \quad \Phi_n^{m'} = 2^{-\frac{1}{2}(2+m)}\phi_n^m, \quad \dot{\Phi}_n^{m'} = 2^{-\frac{1}{2}(3+m)}\dot{\phi}_n^m,$$

$$\sigma' = 2^{\frac{1}{2}}\sigma, \quad \sigma^{0'} = 2^{-\frac{1}{2}}\sigma^0, \quad \dot{\sigma}^{0'} = \tfrac{1}{2}\dot{\sigma}^0, \quad \ddot{\sigma}^{0'} = 2^{-\frac{3}{2}}\ddot{\sigma}^0,$$

$$\rho' = 2^{\frac{1}{2}}\rho, \quad \tau' = \tau, \quad \alpha' = \alpha, \quad \alpha^{0'} = 2^{-\frac{1}{2}}\alpha^0, \quad \beta' = \beta,$$

$$\gamma' = 2^{-\frac{1}{2}}\gamma, \quad \lambda' = 2^{-\frac{1}{2}}\lambda, \quad \mu' = 2^{-\frac{1}{2}}\mu, \quad \nu' = \tfrac{1}{2}\nu,$$

$$\xi^{i'} = \xi^i, \quad X^{i'} = 2^{-\frac{1}{2}}X^i, \quad \omega' = 2^{-\frac{1}{2}}\omega, \quad U' = \tfrac{1}{2}U.$$

[5] E. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962); **4**, 998 (1963).

[6] B. Kozarzewski, Acta Phys. Polon. **27**, 775 (1965).

$$\psi_3 = \psi_3^0 \mathfrak{r}^{-2} + (\bar{\eth}\psi_2^0 + \bar{\phi}_1^0\phi_2^0)\mathfrak{r}^{-3} + O(\mathfrak{r}^{-4}), \quad (5)$$

$$\psi_4 = \psi_4^0 \mathfrak{r}^{-1} + (\bar{\eth}\psi_3^0)\mathfrak{r}^{-2} + O(\mathfrak{r}^{-3}), \quad (6)$$

$$\phi_1 = \phi_1^0 \mathfrak{r}^{-2} + \bar{\eth}\phi_0^0 \mathfrak{r}^{-3} + O(\mathfrak{r}^{-4}), \quad (7)$$

$$\phi_2 = \phi_2^0 \mathfrak{r}^{-1} + \bar{\eth}\phi_1^0 \mathfrak{r}^{-2} + O(\mathfrak{r}^{-3}), \quad (8)$$

$$\rho = -\mathfrak{r}^{-1} - \sigma^0\bar{\sigma}^0\mathfrak{r}^{-3} + O(\mathfrak{r}^{-5}), \quad (9)$$

$$\sigma = \sigma^0\mathfrak{r}^{-2} + (\bar{\sigma}^0\sigma^{0^2} - \tfrac{1}{2}\psi_0^0)\mathfrak{r}^{-4} + O(\mathfrak{r}^{-5}), \quad (10)$$

$$\alpha = \alpha^0\mathfrak{r}^{-1} + \bar{\sigma}^0\bar{\alpha}^0\mathfrak{r}^{-2} + \sigma^0\bar{\sigma}^0\alpha^0\mathfrak{r}^{-3} + O(\mathfrak{r}^{-4}), \quad (11)$$

$$\beta = -\bar{\alpha}^0\mathfrak{r}^{-1} - \sigma^0\alpha^0\mathfrak{r}^{-2} - (\sigma^0\bar{\sigma}^0\bar{\alpha}^0 + \tfrac{1}{2}\psi_1^0)\mathfrak{r}^{-3} + O(\mathfrak{r}^{-4}), \quad (12)$$

$$\tau = -\tfrac{1}{2}\psi_1^0\mathfrak{r}^{-3} + \tfrac{1}{3}(\tfrac{1}{2}\sigma^0\bar{\psi}_1^0 - \bar{\eth}\psi_0^0 - 4\phi_0^0\bar{\phi}_1^0)\mathfrak{r}^{-4} + O(\mathfrak{r}^{-5}), \quad (13)$$

$$\lambda = \dot{\bar{\sigma}}^0\mathfrak{r}^{-1} + \bar{\sigma}^0\mathfrak{r}^{-2} + (\sigma^0\dot{\bar{\sigma}}^0\bar{\sigma}^0 + \tfrac{1}{2}\bar{\sigma}^0\psi_2^0 - \tfrac{1}{2}\bar{\phi}_0^0\phi_2^0)\mathfrak{r}^{-3} + O(\mathfrak{r}^{-4}), \quad (14)$$

$$\mu = -\mathfrak{r}^{-1} - (\sigma^0\dot{\bar{\sigma}}^0 + \psi_2^0)\mathfrak{r}^{-2} - (\sigma^0\bar{\sigma}^0 + \tfrac{1}{2}\bar{\eth}\psi_1^0 + \phi_1^0\bar{\phi}_1^0)\mathfrak{r}^{-3} + O(\mathfrak{r}^{-4}), \quad (15)$$

$$\gamma = -\tfrac{1}{2}\psi_2^0\mathfrak{r}^{-2} - \tfrac{1}{6}(2\bar{\eth}\psi_1^0 - \alpha^0\psi_1^0 + \bar{\alpha}^0\bar{\psi}_1^0 + 6\phi_1^0\bar{\phi}_1^0)\mathfrak{r}^{-3} + O(\mathfrak{r}^{-4}), \quad (16)$$

$$\nu = -\dot{\psi}_3^0\mathfrak{r}^{-1} - (\tfrac{1}{2}\bar{\eth}\psi_2^0 + \bar{\phi}_1^0\phi_2^0)\mathfrak{r}^{-2} + O(\mathfrak{r}^{-3}), \quad (17)$$

$$U = -1 - \tfrac{1}{2}(\psi_2^0 + \bar{\psi}_2^0)\mathfrak{r}^{-1} - \tfrac{1}{6}(\bar{\eth}\psi_1^0 + \eth\bar{\psi}_1^0 + 6\phi_1^0\bar{\phi}_1^0)\mathfrak{r}^{-2} + O(\mathfrak{r}^{-3}), \quad (18)$$

$$X^3 + iX^4\sin\theta = \tfrac{1}{3}\psi_1^0\mathfrak{r}^{-3} + O(\mathfrak{r}^{-4}), \quad (19)$$

X^3 and X^4 being real,

$$\xi^3 = \mathfrak{r}^{-1} - \sigma^0\mathfrak{r}^{-2} + \sigma^0\bar{\sigma}^0\mathfrak{r}^{-3} + O(\mathfrak{r}^{-4}), \quad (20a)$$

$$-i\xi^4\sin\theta = \mathfrak{r}^{-1} + \sigma^0\mathfrak{r}^{-2} + \sigma^0\bar{\sigma}^0\mathfrak{r}^{-3} + O(\mathfrak{r}^{-4}), \quad (20b)$$

$$\omega = -\bar{\eth}\sigma^0\mathfrak{r}^{-1} + (\sigma^0\eth\bar{\sigma}^0 - \tfrac{1}{2}\psi_1^0)\mathfrak{r}^{-2} + O(\mathfrak{r}^{-3}), \quad (21)$$

where

$$\alpha^0 = -\tfrac{1}{2}\cot\theta, \quad (22)$$

$$\psi_2^0 - \bar{\psi}_2^0 = \bar{\eth}^2\sigma^0 - \eth^2\bar{\sigma}^0 + \bar{\sigma}^0\dot{\sigma}^0 - \dot{\bar{\sigma}}^0\sigma^0, \quad (23)$$

$$\psi_3^0 = \eth\dot{\bar{\sigma}}^0, \quad (24)$$

$$\psi_4^0 = -\ddot{\bar{\sigma}}^0. \quad (25)$$

In the above, the "surfaces at infinity" ($\mathfrak{r} = \infty$, $\mathfrak{u} = \text{const}$) have been chosen to be spheres with the usual angular coordinates θ, φ. [Actually only Eqs. (19), (20), and (22) depend on the choice of angular coordinates.] The $\eth$ notation of Newman–Penrose[7] has also been used. Further terms could easily be calculated. The time development of the solution is determined (with the dot denoting $\partial/\partial\mathfrak{u}$) by

$$\dot{\psi}_0^0 + \eth\psi_1^0 - 3\sigma^0\psi_2^0 - 3\phi_0^0\bar{\phi}_2^0 = 0, \quad (26)$$

$$\dot{\psi}_0^1 - 4\bar{\eth}(\sigma^0\psi_1^0) + \bar{\eth}\eth\psi_0^0 + 4\bar{\phi}_1^0\eth\phi_0^0 - 8\sigma^0\phi_1^0\bar{\phi}_1^0 - 4\phi_0^1\bar{\phi}_2^0 = 0, \quad (27)$$

$$\dot{\psi}_1^0 + \eth\psi_2^0 - 2\sigma^0\psi_3^0 - 2\phi_1^0\bar{\phi}_2^0 = 0, \quad (28)$$

$$\dot{\psi}_2^0 + \eth\psi_3^0 - \sigma^0\psi_4^0 - \phi_2^0\bar{\phi}_2^0 = 0, \quad (29)$$

$$\dot{\phi}_0^0 + \eth\phi_1^0 - \sigma^0\phi_2^0 = 0, \quad (30)$$

$$\dot{\phi}_0^1 + \bar{\eth}\eth\phi_0^0 - 2\bar{\eth}(\sigma^0\phi_1^0) = 0, \quad (31)$$

$$\dot{\phi}_1^0 + \eth\phi_2^0 = 0, \quad (32)$$

and the corresponding equations [see Eqs. (56), (57)] for the remaining $\dot{\psi}_0^m$, $\dot{\phi}_0^m$.

In these equations the quantities ψ_0^m, ϕ_0^m ($m = 0, 1, 2, \cdots$), ψ_1^0, $\psi_2^0 + \bar{\psi}_2^0$, ϕ_1^0, as functions of θ, φ, and the quantities σ^0 and ϕ_2^0 as functions of $\mathfrak{u}$, θ, φ are regarded as the given initial data with the remaining quantities expressed in terms of them. Thus, the data needed to determine a solution of the Einstein–Maxwell equations is the null-surface data for the Einstein vacuum equations together with the null-surface data for the flat-space Maxwell equations.[8] Also, the asymptotic symmetry group is just the Bondi–Metzner–Sachs (B.M.S.) group.[9,7]

We shall make use here of the results established in Ref. 2 on the spin weight of each of the ψ's and ϕ's, the expansion of a spin-weighted quantity in series of spin-s spherical harmonics[7] and some properties of $\eth$. In particular, the relations

$$\int {}_sY_{s,m}\bar{\eth}\eta\, dS = 0 \quad \text{and} \quad \int {}_sY_{s,m}\eth\phi\, dS = 0 \quad (33)$$

will be of great value here, where η is any quantity of spin weight $s + 1$ and ϕ is any quantity of spin weight $-s - 1$ defined on the (θ, φ) sphere and $dS = d\theta\sin\theta\, d\varphi$. [One way to prove Eq. (33) is to integrate by parts and use the fact[7] that $\eth_s\bar{Y}_{s,m} = 0$.]

As an example of the techniques to be used, the generalized Bondi–Sachs mass-loss theorem for the Einstein–Maxwell theory[10,11] can be easily obtained. The expression

$$M = -\int {}_0Y_{0,0}(\psi_2^0 + \sigma^0\dot{\bar{\sigma}}^0)\, dS \quad (34)$$

defines, up to a numerical factor, the Bondi–Sachs

[7] E. Newman and R. Penrose, J. Math. Phys. **7**, 863 (1966).

[8] A. Janis and E. Newman, J. Math. Phys. **6**, 902 (1965).

[9] R. K. Sachs, Phys. Rev. **128**, 2851 (1962).

[10] T. Morgan and J. Winicour, Bull. Am. Phys. Soc. **9**, 424 (1964).

[11] R. Penrose, Phys. Rev. Letters **10**, 66 (1963); in *Relativity, Groups and Topology*, C. DeWitt and B. DeWitt, Eds. (Gordon and Breach, Science Publishers, New York, 1964).

total mass[12,13] at retarded time u. (Of course, ${}_0Y_{0,0} = \frac{1}{2}\pi^{-\frac{1}{2}}$.) This M is real by Eq. (23) since

$$\int {}_0Y_{0,0}\eth^2\bar{\sigma}^0\, dS = 0.$$

From Eq. (29) we get

$$\dot{M} = -\int {}_0Y_{0,0}(\dot{\sigma}^0\dot{\bar{\sigma}}^0 + \phi_2^0\bar{\phi}_2^0)\, dS + \int {}_0Y_{0,0}\eth\psi_3^0\, dS. \quad (35)$$

The last term on the right vanishes (ψ_3^0 having spin weight -1), so if we integrate over u from u_0 to u_1 ($u_1 > u_0$) and use the fact that $\dot{\sigma}^0\dot{\bar{\sigma}}^0 + \phi_2^0\bar{\phi}_2^0$ is nonnegative, we obtain

$$M\Big|_{u_0}^{u_1} \leq 0.$$

The Newman–Unti mass[3]

$$-\int {}_0Y_{0,0}\ \mathrm{Re}\ \psi_2^0\, dS$$

differs from M only when $\dot{\sigma}^0 \neq 0$, so in any transition between states with $\dot{\sigma}^0 = 0$ (e.g., between states stationary in the chosen coordinate system), this mass will likewise decrease.

III. CONSERVATION LAWS

Using Eqs. (31) and (32), we can easily obtain the conservation laws associated with the Maxwell field. To obtain the equation of charge conservation we multiply Eq. (32) by ${}_0Y_{0,0}$ and integrate over the sphere to obtain

$$\frac{d}{du}\int {}_0Y_{0,0}\phi_1^0\, dS = -\int {}_0Y_{0,0}\eth\phi_2^0\, dS. \quad (36)$$

By Eq. (33), the right side of this equation vanishes and we have

$$e \equiv \int {}_0Y_{0,0}\phi_1^0\, dS = \text{const.} \quad (37)$$

This is proportional to the charge ($+i \times$ "magnetic charge"). A similar thing can now be done to Eq. (31), namely, multiply it by ${}_1\bar{Y}_{1,m}$ and integrate over the sphere to obtain

$$\frac{d}{du}\int {}_1\bar{Y}_{1,m}\phi_0^1\, dS = \int {}_1\bar{Y}_{1,m}\bar{\eth}A\, dS, \quad (38)$$

where $A \equiv -\eth\phi_0^0 + 2\sigma^0\phi_1^0$ is a quantity of spin weight 2. Again, by Eq. (33), the right side vanishes and we have

$$F_m \equiv \int {}_1\bar{Y}_{1,m}\phi_0^1\, dS = \text{const.} \quad (39)$$

The real and imaginary parts of F_{-1}, F_0, F_1 are the six conserved quantities for the Maxwell field described earlier,[1,2] which in flat space–time would be associated with the presence of incoming electromagnetic radiation.

One can obtain the ten conserved quantities associated with the gravitational field by considering Eq. (27), which we write as

$$\dot{\psi}_0^1 - 4\bar{\eth}(\sigma^0\psi_1^0) + \bar{\eth}\eth\psi_0^0 + 4R = 0, \quad (40)$$

where

$$R \equiv \phi_1^0\bar{\eth}\phi_0^0 - 2\sigma^0\phi_1^0\bar{\phi}_1^0 - \phi_0^1\bar{\phi}_2^0. \quad (41)$$

We first note that if ϕ is a quantity of nonnegative spin weight s, then a unique inverse to the operation $\bar{\eth}$ can be defined on this quantity if and only if[14]

$$\int {}_s\bar{Y}_{s,m}\phi\, dS = 0. \quad (42)$$

This can be seen by expanding ϕ in a series of spin-s spherical harmonics and using the properties of $\bar{\eth}$. Thus, one can uniquely define

$$\bar{\eth}^{-1}(\phi_1^0 - \bar{E}) \quad \text{and} \quad \bar{\eth}^{-1}(\phi_0^1 - F),$$

where

$$\bar{E} \equiv \bar{e}_0 Y_{0,0} \quad (43)$$

and

$$F \equiv \sum_{m=-1}^{+1} F_m\, {}_1Y_{1,m}. \quad (44)$$

The explicit expression for these quantities in an expansion in spin-s spherical harmonics is

$$\bar{\eth}^{-1}(\phi_1^0 - \bar{E}) = -\sum_{l=1}^{\infty}\sum_{m=-l}^{l}\frac{\alpha_{lm}}{[l(l+1)]^{\frac{1}{2}}}\,{}_1Y_{l,m} \quad (45)$$

and

$$\bar{\eth}^{-1}(\phi_0^1 - F) = -\sum_{l=2}^{\infty}\sum_{m=-l}^{l}\frac{\beta_{lm}}{[(l-1)(l+2)]^{\frac{1}{2}}}\,{}_2Y_{l,m}, \quad (46)$$

where

$$\alpha_{lm} \equiv \int {}_0\bar{Y}_{l,m}\phi_1^0\, dS$$

[12] H. Bondi, M. G. J. van der Burg, and A. W. K. Metzner, Proc. Roy. Soc. (London) **A269**, 21 (1962).

[13] R. K. Sachs, Proc. Roy. Soc. (London) **A270**, 103 (1962).

[14] More generally, for an *arbitrary* ϕ, we can define linear operators $\eth^\dagger$ and $\bar{\eth}^\dagger$—the "*generalized inverses*" of $\eth$, $\bar{\eth}$, respectively—by

$$\eth_s^\dagger Y_{l,m} = (l-s+1)^{-\frac{1}{2}}(l+s)^{-\frac{1}{2}}_{s-1}Y_{l,m}, \quad \text{if } -s < l,$$
$$= 0, \quad \text{if } -s = l,$$
$$\bar{\eth}_s^\dagger Y_{l,m} = -(l-s)^{-\frac{1}{2}}(l+s+1)^{-\frac{1}{2}}_{s+1}Y_{l,m}, \quad \text{if } s < l,$$
$$= 0, \quad \text{if } s = l.$$

These satisfy $\eth\eth^\dagger\eth \equiv \eth$, $\eth^\dagger\eth\eth^\dagger \equiv \eth^\dagger$, $\eth^\dagger\eth \equiv \bar{\eth}\bar{\eth}^\dagger$, $\eth\eth^\dagger \equiv \bar{\eth}^\dagger\bar{\eth}$, $\bar{\eth}\bar{\eth}^\dagger\bar{\eth} \equiv \bar{\eth}$, $\bar{\eth}^\dagger\bar{\eth}\eth^\dagger \equiv \bar{\eth}^\dagger$. [Compare R. Penrose, Proc. Cambridge Phil. Soc. **51**, 406 (1955), for the case of matrix generalized inverses.] The expressions $\bar{\eth}^{-1}(\phi_1^0 - \bar{E})$ and $\bar{\eth}^{-1}(\phi_0^1 - F)$ used here can then be written concisely as $\bar{\eth}^\dagger\phi_1^0$ and $\bar{\eth}^\dagger\phi_0^1$.

and

$$\beta_{lm} \equiv \int {}_1\bar{Y}_{l,m}\phi_0^1\, dS.$$

Using these results and also Eqs. (31), (32), and (41), we obtain

$$R = \frac{d}{du}\,[F\bar{\eth}^{-1}(\bar{\phi}_1^0 - \bar{E}) - \bar{\phi}_1^0\bar{\eth}^{-1}(\phi_0^1 - F)] - \bar{\eth}[\bar{\phi}_2^0\bar{\eth}^{-1}(\phi_0^1 - F)]. \quad (47)$$

Then Eq. (40) can be rewritten as

$$\frac{d}{du}\,[\psi_0^1 + 4F\bar{\eth}^{-1}(\bar{\phi}_1^0 - \bar{E}) - 4\bar{\phi}_1^0\bar{\eth}^{-1}(\phi_0^1 - F)] = \bar{\eth}Q, \quad (48)$$

where Q stands for an expression of spin weight 3. Hence, by Eq. (33), if we multiply by ${}_2\bar{Y}_{2,m}$ and integrate over the sphere, we obtain

$$G_m \equiv \int {}_2\bar{Y}_{2,m}[\psi_0^1 + 4F\bar{\eth}^{-1}(\bar{\phi}_1^0 - \bar{E}) - 4\bar{\phi}_1^0\bar{\eth}^{-1}(\phi_0^1 - F)]\, dS = \text{const.} \quad (49)$$

The real and imaginary parts of G_{-2}, G_{-1}, G_0, G_1, G_2 thus define ten conserved quantities for asymptotically flat Einstein–Maxwell fields. They are the same as the N–P gravitationally conserved quantities when the Maxwell field vanishes. Note that we can rewrite (49) in the alternative form

$$G_m \equiv \int {}_2\bar{Y}_{2,m}[\psi_0^1 + 4\phi_0^1\bar{\eth}^{-1}(\bar{\phi}_1^0 - \bar{E}) - 4\bar{E}\bar{\eth}^{-1}(\phi_0^1 - F)]\, dS; \quad (50)$$

the difference in the integrands in (49) and (50) being of the form ${}_2\bar{Y}_{2,m}\bar{\eth}(\bar{\eth}^{-1}A\bar{\eth}^{-1}B)$. If we add (49) to (50), we get a third, more symmetrical, expression

$$G_m \equiv \int {}_2\bar{Y}_{2,m}[\psi_0^1 + 2(\phi_0^1 + F)\bar{\eth}^{-1}(\bar{\phi}_1^0 - \bar{E}) - 2(\bar{\phi}_1^0 + \bar{E})\bar{\eth}^{-1}(\phi_0^1 - F)]\, dS. \quad (51)$$

The quantities G_m, F_m are invariant also under the *supertranslations* of the B.M.S. group. This does not follow from the argument given above, but the result can be obtained by use of an alternative technique.[15,2] The full details of this argument will be given elsewhere; in the case of F_m, the argument is given in its essentials in Ref. 2. For part of the argument of the next section, we shall, in fact, require this supertranslation invariance of the G_m and F_m, so we shall have to *assume* this result here.

[15] R. Penrose, in *Relativity Theory and Astrophysics*, J. Ehlers, Ed. (American Mathematical Society, Providence, R.I., 1967), Vol. VIII.

We propose to establish a connection between the G_m, F_m and multipole moments of the fields in stationary states. This will then define "selection rules" for transitions between such states. Now, by an argument given in Ref. 2, we can show that, for any stationary system, allowable coordinates can be chosen so that $\sigma^0 = 0$ and for which there is no u dependence. Then we shall have $\phi_2^0 = 0$ [see Eq. (29)]. We can always obtain such coordinates by applying a B.M.S. transformation to the coordinates of any allowable N–U stationary system. (This may involve a supertranslation, however, so that the indentification of the F_m, G_m strictly requires their aforementioned supertranslation invariance.) Equations (31) and (30) now become

$$\bar{\eth}\eth\phi_0^0 = 0, \quad \text{whence} \quad \eth\phi_0^0 = 0, \quad \eth\phi_1^0 = 0. \quad (52)$$

These can be immediately integrated, yielding

$$\phi_0^0 = \sum_{m=-1}^{+1} A_m\, {}_1Y_{1,m}, \qquad \phi_1^0 = e\, {}_0Y_{0,0}. \quad (53)$$

Now, using this result, Eqs. (28), (27), and (26) become

$$\eth\psi_2^0 = 0, \quad \bar{\eth}\eth\psi_0^0 = 0, \quad \text{whence} \quad \eth\psi_0^0 = 0, \quad \eth\psi_1^0 = 0, \quad (54)$$

which integrate to

$$\psi_2^0 = -M\, {}_0Y_{0,0} = \bar{\psi}_2^0, \qquad \psi_0^0 = \sum_{m=-2}^{+2} B_m\, {}_2Y_{2,m}, \qquad \psi_1^0 = \sum_{m=-1}^{+1} C_m\, {}_1Y_{1,m}. \quad (55)$$

In order to determine the angular dependence of ψ_0^1 and ϕ_0^1, it is necessary to obtain the equations for the time development of ψ_0^2 and ϕ_0^2. This can be done by a straightforward but tedious calculation along the same lines as was used to obtain Eqs. (26) to (32), yielding

$$\dot{\psi}_0^2 = -\tfrac{1}{2}[\bar{\eth}\eth\psi_0^1 + 6\psi_0^1 + 15\psi_0^0\psi_2^0 - 10\psi_1^0\psi_1^0 + 6\bar{\phi}_1^0\eth\phi_0^1 - 2\bar{\alpha}^0\bar{\phi}_0^0\eth\phi_0^0] + \Omega, \quad (56)$$

where Ω is a quantity that vanishes when

$$\sigma^0 = \phi_2^0 = 0$$

and

$$\dot{\phi}_0^2 = -\tfrac{1}{2}[\bar{\eth}\eth\phi_0^1 + 4\phi_0^1 + 3(\psi_2^0 + \bar{\psi}_2^0)\phi_0^0 - 4\psi_1^0\phi_1^0] + \Pi, \quad (57)$$

where Π is a quantity that vanishes when $\sigma^0 = \phi_0^2 = 0$.

In the stationary case with the above choice of coordinates, Eq. (57) yields

$$\bar{\eth}\eth\phi_0^1 + 4\phi_0^1 = 4\psi_1^0\phi_1^1 - 6\psi_2^0\phi_0^0. \tag{58}$$

This can be integrated by noting that the right side can be expressed as a sum over ${}_1Y_{1,m}$ and then using the properties of $\bar{\eth}\eth$ on a quantity of spin weight 1 to obtain

$$\phi_0^1 = \sum_{m=-2}^{+2} D_m\, {}_1Y_{2,m} + H, \tag{59}$$

where

$$H = \phi_1^0\psi_1^0 - \tfrac{3}{2}\psi_2^0\phi_0^0.$$

The Maxwell conserved quantities are

$$F_m = \int {}_1\bar{Y}_{1,m} H\, dS \tag{60}$$

[and, in fact, $H = F$; see (44)].

The e, C_m, M, and A_m are, respectively, proportional to the electric ($+i \times$ magnetic) charge, mass dipole moment ($+i \times$ angular momentum), mass, and electric ($+i \times$ magnetic) dipole moment. Thus for stationary fields, the Maxwell conserved quantities are explicit quadratic expressions in these 4 moments. (In fact, essentially: mass $\times$ electric dipole $-$ charge $\times$ gravitational dipole; this being an origin-independent expression.)

Finally, to obtain an expression for ψ_0^1 in stationary states, we use Eq. (56) (noting that $\eth\phi_0^0 = 0$) to obtain

$$\bar{\eth}\eth\psi_0^1 + 6\psi_0^1 = 10(\psi_1^0)^2 - 15\psi_0^0\psi_2^0 - 6\bar{\phi}_1^0\eth\phi_0^1. \tag{61}$$

This can be integrated by noting that the right side can be expressed as a sum over ${}_2Y_{2,m}$ and using the properties of $\bar{\eth}\eth$ to obtain

$$\psi_0^1 = \sum_m J_m\, {}_2Y_{3,m} + \tfrac{5}{3}(\psi_1^0)^2 - \tfrac{5}{2}\psi_0^0\psi_2^0 - \bar{\phi}_1^0\eth\phi_0^1. \tag{62}$$

We can now use these expressions to evaluate the conserved quantities in stationary states. From Eqs. (45) and (46) we have that in stationary states

$$\bar{\eth}^{-1}(\bar{\phi}_1^0 - \bar{E}) = 0$$

and

$$\bar{\eth}^{-1}(\phi_0^1 - F) = -\tfrac{1}{2}\sum_m D_m\, {}_2Y_{2,m} = -\tfrac{1}{4}\eth\phi_0^1 \tag{63}$$

and, thus, Eq. (51) becomes

$$G_m = \int {}_2\bar{Y}_{2,m}\{\psi_0^1 + \bar{\phi}_1^0\eth\phi_0^1\}\, dS, \tag{64}$$

which yields by Eq. (62)

$$G_m = \int {}_2\bar{Y}_{2,m} K\, dS, \tag{65}$$

where

$$K = \tfrac{5}{3}(\psi_1^0)^2 - \tfrac{5}{2}\psi_0^0\psi_2^0.$$

Thus, in stationary states, the conserved quantities can be expressed as exactly the same combination of the mass, dipole moment, and quadrupole moment as in the gravitational case. This means that the implied selection rules for the transitions between stationary states of the Einstein–Maxwell field are the same as those between stationary states of the vacuum gravitational field but with additional selection rules imposed by the Maxwell conserved quantities [Eq. (60)]. Whether or not transitions between exactly stationary states[16] are possible at all, however, even when K and H are both unaltered, remains an open question at present.

[16] It seems unlikely that transitions between two different states can ever be achieved if each is to be without time dependence and with $\sigma^0 = 0$ in the *same* coordinate system. This is indicated by some work of Unti on axially symmetric vacuum fields. Thus, it is important that we have supertranslation invariance for the F_m and G_m, for the above selection rules to have any content.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

On the Wigner Supermultiplet Scheme*

K. T. HECHT AND SING CHIN PANG†
Physics Department, University of Michigan, Ann Arbor, Michigan

(Received 22 November 1968)

Calculation of Wigner and Racah coefficients for the group $SU(4) \supset [SU(2) \times SU(2)]$ make it possible to perform the spin–isospin sums in the cfp (fractional parentage coefficients) expansion of the matrix elements of one- and two-body operators in the Wigner supermultiplet scheme. The $SU(4)$ coefficients needed to evaluate one- and two-particle cfp's, the matrix elements of one-body operators, and the diagonal matrix elements of two-body operators are calculated in general algebraic form for many-particle states characterized by the $SU(4)$ irreducible representations $[yy0]$, $[y\,y-1\,0]$, $[yy1]$, $[y11]$, $[y\,y-1\,y-1]$, $[y10]$, $[yy\,y-1]$, $[y00]$, and $[yyy]$, whose states are specified completely by the spin and isospin quantum numbers (y = arbitrary integer). Applications are made to the calculation of the matrix elements of the complete space-scalar part of the Coulomb interaction and the space-scalar part of the particle–hole interaction for nucleons in different major oscillator shells.

1. INTRODUCTION

Since the decomposition of a many-nucleon wavefunction into its space times its spin–isospin part forms a good starting basis for shell-model calculations for many nuclei up to and through the first half of the $2s$, $1d$ shell, a detailed study of the Wigner supermultiplet scheme may still be in order, more than 30 years after the classic work[1] of Wigner, in which he first introduced the concept of spin–isospin supermultiplets and classified the many-nucleon spin–isospin wavefunctions according to the irreducible representations of the group $SU(4)$. The recognition that the spin–isospin part of the one- and several-particle fractional parentage coefficients (cfp)[2] can be identified with simple Wigner coefficients for the group $SU(4)$ leads to the possibility of performing spin–isospin cfp sums in a general way. In all nuclear matrix elements, the dependence on the Wigner supermultiplet quantum numbers, total spin, and isospin can thus be expressed directly by factors which are given simply in terms of $SU(4)$ Wigner and Racah coefficients. Because of recent general interest in the unitary groups, much detailed work[3-5] has been carried out on the groups $U(n)$. In particular, Biedenharn and Louck[3] have shown that complete algebraic formulas for the matrix elements of elementary operators (needed for the calculation of many-particle cfp's) can be read off at once from patterns assigned to these operators by means of a so-called pattern calculus. Unfortunately, these results cannot be applied to the Wigner supermultiplet scheme, since they apply only if the symmetry classification is given by the canonical chain of unitary groups, such as $U(4) \supset U(3) \supset U(2) \supset U(1)$. (In the classification scheme based on a canonical chain of subgroups, the states of a given irreducible representation are completely specified by the representation labels of all the subgroups in the chain.) Unfortunately, the group chains of actual physical interest in spectroscopy rarely coincide with these mathematically natural or canonical chains. In the Wigner supermultiplet classification, the physics dictates that the representations of $SU(4)$ be reduced according to the subgroup $SU(2) \times SU(2)$, where the direct product of the two $SU(2)$ groups is generated by the commuting spin and isospin operators. Neither of these is related to the group $U(2)$ in the canonical chain. Since the group $SU(4)$ and the 6-dimensional rotation group $O(6)$ have Lie algebras of identical structure, the Wigner supermultiplet scheme can also be considered from the point of view of the group $O(6)$. The canonical group chain $O(6) \supset O(5) \supset O(4) \supset O(3) \supset O(2)$ is again not the physically relevant one. Although *either* ordinary spin *or* isospin can be put into correspondence with the representations of the group $O(3)$ in this chain, the other is not a good quantum number in this canonical classification scheme for $O(6)$. The calculation of the needed supermultiplet Wigner coefficients must thus proceed from the specific properties of the group chain $SU(4) \supset [SU(2) \times SU(2)]$. Such calculations are complicated by the state-labeling problem. In the most general irreducible representation of $SU(4)$, the states are not completely specified by the spin and isospin quantum numbers alone. Although the additional operators needed for a complete classification of the states of a supermultiplet have been constructed

* Supported by the U.S. Office of Naval Research, Contract Nonr. 1224(59).

† Present address: Physics Dept., University of Pennsylvania, Philadelphia, Pennsylvania.

[1] E. P. Wigner, Phys. Rev. **51**, 106 (1937).

[2] H. A. Jahn and H. van Wieringen, Proc. Roy. Soc. (London) **A209**, 502 (1951).

[3] L. C. Biedenharn and J. D. Louck, Commun. Math. Phys. **8**, 89 (1968).

[4] M. Moshinsky, in *Group Theory and the Many Body Problem*, E. Meeron, Ed. (Gordon and Breach, Science Publishers, New York, 1966).

[5] P. Carruthers, *Introduction to Unitary Symmetry* (Interscience Publishers, Inc., New York, 1966).

by Moshinsky and Nagel,[6] the algebraic structure of the eigenvectors associated with such operators is rather complicated and makes it very difficult to derive general algebraic formulas for the Wigner coefficients for the group $SU(4) \supset [SU(2) \times SU(2)]$, valid for all irreducible representations.[7] With relatively few exceptions, however, the $SU(4)$ representations of practical importance for shell-model calculations can be shown to fall into a few simple classes in which states of a given spin–isospin (S, T) occur at most once. By restricting the discussion to those irreducible representations in which all states are specified completely by the spin and isospin quantum numbers, it is possible to give general algebraic formulas for the $SU(4)$ Wigner and Racah coefficients needed to exploit to the fullest the properties of the group $SU(4)$ in the study of nuclei. By restricting the irreducible representations to those of the above type, a further simplification is achieved in connection with the multiplicity problem associated with the fact that Kronecker products of two $SU(4)$ representations are, in general, not simply reducible. For the irreducible representations of the above type and the Kronecker products which occur in nuclear model calculations, these multiplicities are never greater than two.

Our general approach is similar to that of a recent contribution by Kukulin, Smirnov, and Majling[8] on the Racah algebra of $SU(4)$. However, the aim of the present work is quite different insofar as it attempts to give explicit formulas, in general algebraic form, for most of the $SU(4)$ coefficients needed in shell model studies. The aim is not only to facilitate calculations but to derive explicit algebraic formulas which make it possible to study general trends in the dependence of nuclear matrix elements on the Wigner supermultiplet, spin, and isospin quantum numbers.

To establish the notation, a review of the properties of $SU(4)$ and the supermultiplet scheme is given in Sec. 2. In Sec. 3 the irreducible representations which are completely specified by the spin and isospin quantum numbers are identified. Explicit constructions are given for their state vectors in terms of a sequence of step-down operators acting on the state of highest weight. In Sec. 4 the general properties of the $SU(4)$ Wigner and Racah coefficients are discussed together with the methods used in the actual calculation of the coefficients required for shell-model studies. Tabulations are given in a set of appendices. Some applications are given in Sec. 5. Since the discussion is restricted to the spin–isospin parts of the many-nucleon wavefunctions, the detailed applications necessarily involve the discussion of physical operators which can be approximated by their complete space-scalar parts. The Coulomb interaction, for example, is rather insensitive to the details of the space parts of the wavefunctions. Matrix elements of the space-scalar part of the Coulomb interaction are calculated in Sec. 5 in order to study the dependence of the Coulomb energy on the Wigner supermultiplet, spin, and isospin quantum numbers.[9] Since a space-scalar approximation to the particle–hole interaction may give a good estimate of the full particle–hole interaction energy in $2s, 1d$ shell nuclei,[10] matrix elements for such a particle–hole interaction are derived in general algebraic form through the $SU(4)$ Wigner coefficients which are tabulated in the appendices. Even if an operator cannot be approximated by its complete space-scalar part, the full expression for its matrix elements in terms of cfp expansions can be simplified since the spin–isospin part of the cfp sum can be performed so that the over-all dependence on $[f]$, S, and T is given by the $SU(4)$ Wigner and Racah coefficients of the type tabulated in the appendices. By extending these techniques to the unitary groups needed to classify the space parts of the wavefunctions, the full cfp expansions can in principle be summed in general. The resultant interplay between the supermultiplet and spatial quantum numbers will be discussed in a future publication.

2. PROPERTIES OF $SU(4)$ AND THE SUPERMULTIPLET SCHEME

2.1. Infinitesimal Operators

The supermultiplet scheme is based on the four spin–charge states of a single nucleon $|m_s m_t\rangle$. These are

$$|1\rangle = |+\tfrac{1}{2}\,+\tfrac{1}{2}\rangle, \quad |2\rangle = |+\tfrac{1}{2}\,-\tfrac{1}{2}\rangle,$$
$$|3\rangle = |-\tfrac{1}{2}\,+\tfrac{1}{2}\rangle, \quad |4\rangle = |-\tfrac{1}{2}\,-\tfrac{1}{2}\rangle. \qquad (1)$$

(Note that the first label indicates the spin, the second the isospin quantum number.) These states can also be expressed in terms of the single nucleon-creation operators $a^{\dagger}_{\alpha i}$, where α stands for the full set of space-quantum numbers, e.g., $\alpha = nlm_l$, and $i = 1, 2, 3$, or 4 stands for the spin–isospin quantum numbers $m_s m_t$ in the sense of Eq. (1), such that $|\alpha, i\rangle = a^{\dagger}_{\alpha i}|0\rangle$. The infinitesimal operators which generate the unitary transformations in the 4-dimensional space can be built from these fermion creation operators and their

[6] M. Moshinsky and J. G. Nagel, Phys. Letters **5**, 173 (1963).
[7] See M. Resnikoff, preprint, SUNY at Buffalo (1968).
[8] V. I. Kukulin, Yu. F. Smirnov, and L. Majling, Nucl. Phys. **A103**, 681 (1967).
[9] K. T. Hecht, Nucl. Physics **A114**, 280 (1968).
[10] K. T. Hecht, P. J. Ellis, and T. Engeland, Phys. Letters **27B**, 479 (1968).

TABLE I. The infinitesimal operators (Infin. ops.).

Infin. ops.	$SU(4)$ generators	$O(6)$ generators	$SU(4)$ irreducible tensor components (standard phases) $T^{[f]}_{(SM_S)(TM_T)}$
S_0	$\frac{1}{2}(A_{11}+A_{22}-A_{33}-A_{44})$	J_{12}	$T^{[211]}_{(10)(00)}$
T_0	$\frac{1}{2}(A_{11}-A_{22}+A_{33}-A_{44})$	J_{56}	$T^{[211]}_{(00)(10)}$
$E_{00}(Y)$	$\frac{1}{2}(A_{11}-A_{22}-A_{33}+A_{44})$	J_{34}	$-T^{[211]}_{(00)(00)}$
S_+	$(1/\sqrt{2})(A_{13}+A_{24})$	$(1/\sqrt{2})(J_{13}+iJ_{23})$	$-T^{[211]}_{(11)(00)}$
S_-	$(1/\sqrt{2})(A_{31}+A_{42})$	$(1/\sqrt{2})(J_{13}-iJ_{23})$	$T^{[211]}_{(1-1)(00)}$
T_+	$(1/\sqrt{2})(A_{12}+A_{34})$	$(1/\sqrt{2})(J_{45}+iJ_{46})$	$-T^{[211]}_{(00)(11)}$
T_-	$(1/\sqrt{2})(A_{21}+A_{43})$	$(1/\sqrt{2})(J_{45}-iJ_{46})$	$T^{[211]}_{(00)(1-1)}$
E_{10}	$(1/\sqrt{2})(A_{13}-A_{24})$	$(i/\sqrt{2})(J_{14}+iJ_{24})$	$T^{[211]}_{(11)(10)}$
E_{-10}	$(1/\sqrt{2})(A_{31}-A_{42})$	$(-i/\sqrt{2})(J_{14}-iJ_{24})$	$-T^{[211]}_{(1-1)(10)}$
E_{01}	$(1/\sqrt{2})(A_{12}-A_{34})$	$(-i/\sqrt{2})(J_{35}+iJ_{36})$	$T^{[211]}_{(10)(11)}$
E_{0-1}	$(1/\sqrt{2})(A_{21}-A_{43})$	$(i/\sqrt{2})(J_{35}-iJ_{36})$	$-T^{[211]}_{(10)(1-1)}$
E_{11}	A_{14}	$\frac{1}{2}[(J_{15}+iJ_{25})+i(J_{16}+iJ_{26})]$	$-T^{[211]}_{(11)(11)}$
E_{-1-1}	A_{41}	$\frac{1}{2}[(J_{15}-iJ_{25})-i(J_{16}-iJ_{26})]$	$-T^{[211]}_{(1-1)(1-1)}$
E_{1-1}	A_{23}	$\frac{1}{2}[-(J_{15}+iJ_{25})+i(J_{16}+iJ_{26})]$	$T^{[211]}_{(11)(1-1)}$
E_{-11}	A_{32}	$\frac{1}{2}[-(J_{15}-iJ_{25})-i(J_{16}-iJ_{26})]$	$T^{[211]}_{(1-1)(11)}$

conjugate annihilation operators:

$$A_{ij}=\sum_{\alpha} a^{\dagger}_{\alpha i}a_{\alpha j},\quad i,j=1\cdots 4. \tag{2}$$

They contain the three components of the spin operator **S** and the isospin operator **T** together with the nine components of the operator

$$\mathbf{E}=\sum_{\alpha ij}\langle i|\,\boldsymbol{\sigma\tau}\,|j\rangle\, a^{\dagger}_{\alpha i}a_{\alpha j}, \tag{3}$$

where $\boldsymbol{\sigma}$, $\boldsymbol{\tau}$ are the single-particle Pauli spin and isospin operators. As a specific example, let us take

$$\begin{aligned}E_{1-1}&=\sum_{\alpha m_s'\cdots m_t'}\langle m_s'm_t'|\,\sigma_+\tau_-\,|m_sm_t\rangle\, a^{\dagger}_{\alpha m_s'm_t'}a_{\alpha m_sm_t}\\&=\sum_{\alpha}a^{\dagger}_{\alpha\frac{1}{2}-\frac{1}{2}}a_{\alpha-\frac{1}{2}\frac{1}{2}}\\&=A_{23}.\end{aligned} \tag{4}$$

The 15 operators **S**, **T**, and **E** generate the group $SU(4)$. Together with the number operator $N_{\mathrm{op}}=\sum_i A_{ii}$, they generate the full group $U(4)$. The relation between the A_{ij} and the full set of Wigner supermultiplet operators **S**, **T**, **E** is shown in Table I. The components of **S**, **T**, and **E** are all normalized such that the structure constants are ± 1 or 0. The commutation relations for the operators follow from the anticommutation relations of $a^{\dagger}$ and a. They are given by

$$[A_{ij},A_{kl}]=\delta_{jk}A_{il}-\delta_{il}A_{kj}. \tag{5}$$

Since the groups $SU(4)$ and $O(6)$ have Lie algebras of identical structure, the 15 infinitesimal operators can also be expressed in terms of angular-momentum operators J_{ij} $(i,j=1,\cdots,6)$ which generate rotations in a 6-dimensional real space. The specific relationship is shown in Table I. The spin and isospin spaces have been chosen as the (1, 2, 3) and (4, 5, 6) 3-dimensional subspaces of the full 6-dimensional space.

2.2. Irreducible Representations

The irreducible representations of the group $U(4)$ can be specified by the permutation symmetries of the n-nucleon spin–isospin functions. These symmetries are characterized by Young tableaux of 4 rows or partition numbers $[f_1f_2f_3f_4]$ on n objects, where f_i are integers such that $f_1+f_2+f_3+f_4=n$ and $f_1\geq f_2\geq f_3\geq f_4\geq 0$. The partition number f_i specifies the length of the ith row of the Young tableau. Since a totally antisymmetric 4-particle spin–isospin function is invariant under *unimodular* unitary transformations in the 4-dimensional space of the single-particle states, columns of four can be removed from the Young tableaux in restricting the irreducible representations to those of the group $SU(4)$. The irreducible representations of $SU(4)$ are thus specified by 3-rowed Young tableaux or the partition numbers $[f_1-f_4, f_2-f_4, f_3-f_4]$. The irreducible representation labels are often abbreviated by $[f]$. (For economy in writing representations, $[y00]$, $[yy0]$, and $[yyy]$ will sometimes also be denoted by $[y]$, $[y^2]$, and $[y^3]$, respectively.) The irreducible representations of $SU(4)$ can also be specified by the highest weights of the three commuting operators S_0, T_0, E_{00} of the rank 3 group. In an n-particle spin–isospin function of the

above symmetry, there can be at most f_1 particles in state $|1\rangle$; of the remaining particles there can be at most f_2 particles in state $|2\rangle$; etc. The highest weights associated with the operators S_0, T_0, E_{00} are thus given by

$$\begin{aligned} P &= \tfrac{1}{2}(f_1 + f_2 - f_3 - f_4), \\ P' &= \tfrac{1}{2}(f_1 - f_2 + f_3 - f_4), \\ P'' &= \tfrac{1}{2}(f_1 - f_2 - f_3 + f_4), \end{aligned} \tag{6}$$

where P = maximum value of S_0 (and therefore S) contained in the representation; P' = maximum value of T_0 for a state having $S_0 = P$; and P'' = maximum value of E_{00} for a state with $S_0 = P$ and $T_0 = P'$. The three supermultiplet quantum numbers (P, P', P'') also specify the $O(6)$ irreducible representations according to the standard Weyl–Gel'fand labeling scheme.[11] (To avoid confusion, $O(6)$ quantum numbers (P, P', P'') will always be enclosed in round parentheses, $SU(4)$ quantum numbers $[f]$ by square brackets.)

2.3. State-Labeling Problem

Since the group $SU(4)$ [or alternately $O(6)$] is a 15-parameter group of rank 3, the states of a given irreducible representation are, in general, specified completely[12] by $\frac{1}{2}(15 - 3)$ or 6 quantum numbers in addition to the irreducible representation labels. The 6 additional quantum numbers could in principle be furnished by the irreducible representation labels of all the subgroups in one of the canonical subgroup chains (Fig. 1). In the chain based on $U(4)$, however, neither the spin nor the isospin operators can be put into correspondence with the subgroup $U(2)$. (Neither can the operators $\mathbf{S}$ nor $\mathbf{T}$ be identified with A_{ij}, $i, j = 1, 2$, or some other pair.) In the chain based on $O(6)$ it is possible to identify m_{31} and m_{21} with *either* the quantum numbers SM_S *or* TM_T. According to the specific choice of Table I, $m_{31} = S$, $m_{21} = M_S$, but in this scheme the operators $\mathbf{T}^2$ and T_0 are not diagonal. A complete classification of the state vectors for $SU(4) \supset [SU(2) \times SU(2)]$ must thus be given by a set of 6 commuting operators which must include, besides $\mathbf{S}^2$, S_0, $\mathbf{T}^2$, T_0, two additional operators. Unfortunately, the eigenvalues of the two additional operators cannot be simply related to irreducible representation labels of a subgroup of $SU(4)$. In the most general irreducible representation of $SU(4)$, the algebraic structure of the eigenvectors associated with these operators is therefore complicated. Moshinsky and Nagel[6] have suggested that the additional operators be chosen as

$$\begin{aligned} \Omega &= S_i E_{ij} T_j, \\ \Phi &= S_i S_j E_{ik} E_{jk} + E_{ki} E_{kj} T_i T_j \\ &\quad - \epsilon_{ijk} \epsilon_{lmn} S_i E_{jm} E_{kn} T_l, \end{aligned} \tag{7}$$

where $i, j, \cdots$ stand for Cartesian components (rather than the spherical ones of Table I) and summation convention is implied by repeated indices. Because of the algebraic difficulties involved in the eigenvalue problem associated with operators such as Ω and Φ, it has not been possible to derive expressions for the Wigner coefficients of the supermultiplet scheme in a completely general way. In actual practice, however, most of the Wigner supermultiplets of importance for shell-model studies fall into a few special classes for which the spin and isospin quantum numbers are sufficient for a complete classification. The present work will be restricted to the study of such irreducible representations. For these the needed $SU(4)$ Wigner and Racah coefficients can be calculated.

$$\begin{array}{cccc} f_1 & f_2 & f_3 & f_4 \\ m_{31} & m_{32} & m_{33} & \\ m_{21} & m_{22} & & \\ m_{11} & & & \end{array} \qquad \begin{array}{ccc} P & P' & P'' \\ m_{51} & m_{52} & \\ m_{41} & m_{42} & \\ m_{31} & & \\ m_{21} & & \end{array}$$

(a) (b)

FIG. 1. Weyl–Gel'fand canonical state labeling schemes based on the group chains (a) $U(4) \supset U(3) \supset U(2) \supset U(1)$ and (b) $O(6) \supset O(5) \supset O(4) \supset O(3) \supset O(2)$. The quantum numbers m_{ni} label the irreducible representations of $U(n)$ in (a) and $O(n)$ in (b). Note that $f_i \equiv m_{4i}$ and $(P, P', P'') \equiv (m_{61}, m_{62}, m_{63})$. The m_{ni} satisfy the branching rule $m_{ni} \leq m_{n-1,i} \leq m_{n,i+1}$. For $U(n)$ the m_{ni} are positive integers. For $O(n)$ they are positive integers or half-integers with the exception of m_{21}, m_{42}, and m_{63}, which may be negative; for these the branching rule becomes $|m_{2k,k}| \leq m_{2k+1,k}$.

2.4. Construction of State Vectors; Step-Up and Step-Down Operators

In the most general irreducible representation of $SU(4)$, the state vectors (or many-particle spin–isospin wavefunctions), can be denoted by

$$|[f]\omega\varphi, SM_S TM_T\rangle, \tag{8}$$

where ω and φ are the eigenvalues of the operators Ω and Φ. In the following sections the discussion will be restricted to those irreducible representations for which all state vectors are uniquely determined by the quantum numbers $SM_S TM_T$. For these the quantum numbers ω and φ are redundant, and the state vectors can be denoted by

$$|[f]SM_S TM_T\rangle. \tag{9}$$

For these representations the full set of state vectors can be constructed by a successive application of step-down operators acting on the state of highest

[11] I. M. Gel'fand, R. A. Minlos, and Z. Ya. Shapiro, *Representations of the Rotation and Lorentz Groups and their Application* (The Macmillan Company, New York, 1963), p. 353.

[12] G. Racah, "Group Theory and Spectroscopy," lecture notes, Princeton (1951); CERN reprint 61-8 (1961).

TABLE II. The step operators $O_{\alpha\beta}$.

$$O_{11} = E_{11}$$

$$O_{01} = E_{01} + S_{-}E_{11}\frac{1}{S_0+1}$$

$$O_{10} = E_{10} + T_{-}E_{11}\frac{1}{T_0+1}$$

$$O_{00} = E_{00} + S_{-}E_{10}\frac{1}{S_0+1} + T_{-}E_{01}\frac{1}{T_0+1} + S_{-}T_{-}E_{11}\frac{1}{(S_0+1)(T_0+1)}$$

$$O_{1-1} = E_{1-1} - T_{-}E_{10}\frac{1}{T_0} - T_{-}^{2}E_{11}\frac{1}{T_0(2T_0+1)}$$

$$O_{-11} = E_{-11} - S_{-}E_{01}\frac{1}{S_0} - S_{-}^{2}E_{11}\frac{1}{S_0(2S_0+1)}$$

$$O_{0-1} = E_{0-1} + S_{-}E_{1-1}\frac{1}{(S_0+1)} - T_{-}E_{00}\frac{1}{T_0} - T_{-}^{2}E_{01}\frac{1}{T_0(2T_0+1)} - S_{-}T_{-}E_{10}\frac{1}{T_0(S_0+1)} - T_{-}^{2}S_{-}E_{11}\frac{1}{(S_0+1)T_0(2T_0+1)}$$

$$O_{-10} = E_{-10} + T_{-}E_{-11}\frac{1}{(T_0+1)} - S_{-}E_{00}\frac{1}{S_0} - S_{-}^{2}E_{10}\frac{1}{S_0(2S_0+1)} - S_{-}T_{-}E_{01}\frac{1}{S_0(T_0+1)} - T_{-}S_{-}^{2}E_{11}\frac{1}{(T_0+1)S_0(2S_0+1)}$$

$$O_{-1-1} = E_{-1-1} - T_{-}E_{-10}\frac{1}{T_0} - S_{-}E_{0-1}\frac{1}{S_0} - T_{-}^{2}E_{-11}\frac{1}{T_0(2T_0+1)} - S_{-}^{2}E_{1-1}\frac{1}{S_0(2S_0+1)} + S_{-}T_{-}E_{00}\frac{1}{S_0T_0} + S_{-}^{2}T_{-}E_{10} \times \frac{1}{S_0(2S_0+1)T_0} + S_{-}T_{-}^{2}E_{01}\frac{1}{S_0T_0(2T_0+1)} + S_{-}^{2}T_{-}^{2}E_{11} \times \frac{1}{S_0T_0(2S_0+1)(2T_0+1)}$$

weight. Since the properties of angular-momentum eigenvectors are well known, it will be sufficient to construct the state vectors with $M_S = S$, $M_T = T$. It will sometimes be convenient to use the short-hand notation (employing curly brackets):

$$|[f]\{ST\}\rangle \equiv |[f]SM_S = S, TM_T = T\rangle. \quad (10)$$

A step operator $O_{\alpha\beta}$ is defined by

$$O_{\alpha\beta}\,|[f]\{ST\}\rangle = N_{\alpha\beta}^{[f]}(S, T)\,|[f]\{S+\alpha, T+\beta\}\rangle, \quad (11)$$

where

$$N_{\alpha\beta}^{[f]}(S, T) = [\langle[f]\{ST\}|\,O_{\alpha\beta}^{\dagger}O_{\alpha\beta}\,|[f]\{ST\}\rangle]^{\frac{1}{2}} = [\langle[f]\{ST\}|\,O_{-\alpha-\beta}O_{\alpha\beta}\,|[f]\{ST\}\rangle]^{\frac{1}{2}} \quad (12)$$

and

$$N_{\alpha\beta}^{[f]}(S, T) = N_{-\alpha-\beta}^{[f]}(S+\alpha, T+\beta). \quad (13)$$

The choice of the positive sign for the normalization factors, Eq. (12), specifies the phase convention used in this investigation. The step operators $O_{\alpha\beta}$ must satisfy the commutation relations

$$[S_+, O_{\alpha\beta}]\,|[f]\{ST\}\rangle = 0,$$
$$[T_+, O_{\alpha\beta}]\,|[f]\{ST\}\rangle = 0. \quad (14)$$

These equations are sufficient to construct the operators. There are 9 basic step operators corresponding to the $9E$ generators. The operators are shown in Table II. [The operators $O_{\alpha\beta}$ are not unique, but the lack of uniqueness can involve only trivial additional factors or combinations. For example, if $O_{\alpha\beta}$ satisfies Eqs. (14), so does $O_{\alpha\beta} + O'T_+$, where O' is any arbitrary operator. The lack of uniqueness in O_{10} can be illustrated by noting that $O_{1-1}O_{01} = O'_{10} \neq O_{10}$.] It will be convenient to express the nine E generators in terms of the O operators. The results are shown in Table III.

2.5. Irreducible Tensor Operators; Tensor Character of the Generators

The 15 infinitesimal operators **S**, **T**, and $\mathbf{E}_{ab}$ transform according to the regular representation [211] and have spin–isospin spherical tensor character $ST = 10$, 01, and 11, respectively.

The components of an $SU(4)$ irreducible tensor operator $T^{[f]}_{(SM_S)(TM_T)}$ can be defined by the commutator equations

$$[E_{ab}, T^{[f]}_{(SM_S)(TM_T)}] = \sum_{S'T'} \langle[f](S'M_S + a)(T'M_T + b)| \times E_{ab}\,|[f](SM_S)(TM_T)\rangle\, T^{[f]}_{(S'M_S+a)(T'M_T+b)} \quad (15)$$

TABLE III. Expressions for the E operators in terms of the O operators.

$$E_{11} = O_{11}$$

$$E_{01} = O_{01} - S_{-}O_{11}\frac{1}{(S_0+1)}$$

$$E_{10} = O_{10} - T_{-}O_{11}\frac{1}{(T_0+1)}$$

$$E_{00} = O_{00} - S_{-}O_{10}\frac{1}{(S_0+1)} - T_{-}O_{01}\frac{1}{(T_0+1)} + S_{-}T_{-}O_{11}\frac{1}{(S_0+1)(T_0+1)}$$

$$E_{1-1} = O_{1-1} + T_{-}O_{10}\frac{1}{T_0} - T_{-}^2O_{11}\frac{1}{(T_0+1)(2T_0+1)}$$

$$E_{-11} = O_{-11} + S_{-}O_{01}\frac{1}{S_0} - S_{-}^2O_{11}\frac{1}{(S_0+1)(2S_0+1)}$$

$$E_{0-1} = O_{0-1} + T_{-}O_{00}\frac{1}{T_0} - S_{-}O_{1-1}\frac{1}{(S_0+1)} - T_{-}S_{-}O_{10}\frac{1}{T_0(S_0+1)} - T_{-}^2O_{01}\frac{1}{(2T_0+1)(T_0+1)} + S_{-}T_{-}^2O_{11}\frac{1}{(S_0+1)(T_0+1)(2T_0+1)}$$

$$E_{-10} = O_{-10} + S_{-}O_{00}\frac{1}{S_0} - T_{-}O_{-11}\frac{1}{(T_0+1)} - T_{-}S_{-}O_{01}\frac{1}{S_0(T_0+1)} - S_{-}^2O_{10}\frac{1}{(2S_0+1)(S_0+1)} + T_{-}S_{-}^2O_{11}\frac{1}{(T_0+1)(S_0+1)(2S_0+1)}$$

$$E_{-1-1} = O_{-1-1} + S_{-}O_{0-1}\frac{1}{S_0} + T_{-}O_{-10}\frac{1}{T_0} + T_{-}S_{-}O_{00}\frac{1}{S_0T_0} - S_{-}^2O_{1-1}\frac{1}{(S_0+1)(2S_0+1)} + T_{-}^2O_{-11}\frac{1}{(T_0+1)(2T_0+1)} - T_{-}^2S_{-}O_{01}\frac{1}{S_0(2T_0+1)(T_0+1)} - T_{-}S_{-}^2O_{10}\frac{1}{T_0(2S_0+1)(S_0+1)} + T_{-}^2S_{-}^2O_{11}\frac{1}{(T_0+1)(S_0+1)(2S_0+1)(2T_0+1)}$$

with the analogous well-known commutator equations involving **S** and **T**; e.g.,

$$[S_a, T^{[f]}_{(SM_S)(TM_T)}] = \langle SM_S + a|\, S_a\, |SM_S\rangle\, T^{[f]}_{(SM_S+a)(TM_T)}. \quad (16)$$

The operators **S**, **T**, and E_{ab} themselves have irreducible tensor character $T^{[211]}$. It is important to determine the phases implied by the standard defining equations (15). The full set of states of the representation [211] can be constructed by the step-down operators O_{0-1} and O_{-10} acting on the highest-weight state with $\{ST\} = \{11\}$. The normalization coefficients (13) are, in this case,

$$N^{[211]}_{0-1}(1,1) = N^{[211]}_{-10}(1,1) = +1. \quad (17)$$

With these and the relations of Table III, the matrix elements of E_{ab} can be evaluated. The relation between the components of **S**, **T**, and **E** and the standard components of the irreducible tensor operator $T^{[211]}$ then follow from Eqs. (15) and (16). The results are shown in the last column of Table I. The over-all phase is fixed so that the components of **S** and **T** have phases according to the standard conventions for spherical tensors. [Note the minus signs for the $SU(4)$ tensor components with $(SM_S)(TM_T) = (11)(00)$ and (00)(11) in Table I.]

2.6. Conjugate Representations

If a many-nucleon spin–isospin wavefunction transforms according to the $SU(4)$ irreducible representation $[f]$, the conjugate of such a function transforms according to the conjugate representation, to be denoted by $[f^*]$, where for

$$[f] = [f_1 - f_4, f_2 - f_4, f_3 - f_4],$$
$$[f^*] = [f_1 - f_4, f_1 - f_3, f_1 - f_2], \quad (18a)$$

or, in terms of the supermultiplet quantum numbers P, P', P'',

$$(P, P', P'')^* \equiv (P, P', -P''). \quad (18b)$$

The conjugate representations $[f^*]$ can be pictured in terms of spin–isospin functions for $n = 3f_1 - f_2 - f_3 - f_4$ nucleons which have been lifted out of a configuration whose Young tableaux are given by $(f_1 - f_4)$ columns of 4—the well-known particle–hole relationship. Note also that the single-nucleon creation operators $a^\dagger$ have tensor character [1], while the annihilation operators a have tensor character [111]. The irreducible representations of $SU(2)$ are self-conjugate. For spherical tensors, conjugation

implies only $M_S \to -M_S$, $M_T \to -M_T$. The conjugate of a state vector is thus given by

$$|[f]SM_S, TM_T\rangle^* = (-1)^{\eta}(-1)^{S-M_S+T-M_T}\ |[f^*]S - M_S, T - M_T\rangle. \tag{19}$$

The phase factor has been split into two pieces: one gives the dependence on the spin–isospin quantum numbers standard for spherical tensor operators; the second, denoted by η, is independent of M_S, M_T, but is a function of S, T, and $[f]$: $\eta = \eta([f], S, T)$. The phase factors for the representations of interest in this investigation are evaluated in Sec. 3. The dependence on $[f]$ is a matter of arbitrary phase conventions. The choice of phase conventions adopted in this work (Sec. 3) is such that the irreducible tensor character of the single-nucleon creation and annihilation operators is given by

$$a^{\dagger}_{\alpha m_s m_t} \to T^{[1]}_{(\frac{1}{2}m_s)(\frac{1}{2}m_t)},$$
$$a_{\alpha m_s m_t} \to (-1)^{\frac{1}{2}-m_s+\frac{1}{2}-m_t} T^{[111]}_{(\frac{1}{2}-m_s)(\frac{1}{2}-m_t)}. \tag{20}$$

In addition, the operators **S** and **T** are to have the conjugation properties standard for ordinary spherical tensor operators. This implies

$$(-1)^{\eta([211]1,0)} = (-1)^{\eta([211]0,1)} = +1. \tag{21}$$

2.7. Casimir Invariant

The quadratic Casimir operator is of particular importance. It can be expressed as

$$\mathbf{C} = \sum_{i<j=1}^{6} J_{ij}^2 = \sum_{ab} E_{ab}E_{ba} + \mathbf{S}^2 + \mathbf{T}^2. \tag{22a}$$

This can be brought into the form

$$\mathbf{C} = 2(E_{-1-1}E_{11} + E_{-11}E_{1-1} + E_{-10}E_{10} + E_{0-1}E_{01} + S_-S_+ + T_-T_+) + S_0^2 + 4S_0 + T_0^2 + 2T_0 + E_{00}^2, \tag{22b}$$

from which the eigenvalue of the Casimir operator can be read off by acting on the state of highest weight with $S_0 = P$, $T_0 = P'$, $E_{00} = P''$. This gives the Casimir invariant

$$C(SU_4) = P(P + 4) + P'(P' + 2) + P''^2. \tag{23}$$

2.8. Kronecker Products

The Kronecker product of two irreducible representations of $U(4)$ is given by the Littlewood rules for outer multiplication of $[f]$-symmetric states.[13]

The one-and two-particle coefficients of fractional parentage are simply related to the matrix elements of $a^{\dagger}$ (or a) and $a^{\dagger}a^{\dagger}$ (or aa), respectively. These coefficients are therefore related to the coupling coefficients for the products $[f_1] \times [f_2]$, where $[f_1]$ is the representation for an arbitrary n-nucleon spin–isospin symmetry, and $[f_2]$ is a one-particle (or hole), or two-particle (or two-hole) representation; that is, $[f_2] = [1]$ (or $[1^3]$); or the antisymmetrically coupled two-particle representation $[1^2]$ (which is self-conjugate), or the symmetrically coupled two-particle representation [2] (or its conjugate $[2^3]$). All such products are simply reducible. In addition to these, the Kronecker products of particular interest for nuclear physics applications are those needed for the evaluation of matrix elements of the one-body operators $(a^{\dagger}a)$ and the two-body operators $(a^{\dagger}a^{\dagger}aa)$. From the reduction of the Kronecker product

$$[1] \times [1^3] = [0] + [211], \tag{24}$$

it can be seen that the one-body operators are either $SU(4)$ scalars or [211] tensors. Similarly, from the reduction of the products

$$[11] \times [11] = [0] + [211] + [22],$$
$$[2] \times [2^3] = [0] + [211] + [422], \tag{25}$$

it can be seen that the two-body operators transform according to the representations [0], [211], [22], and [422]. [Products involving symmetrically coupled pair-creation operators with antisymmetrically coupled pair-annihilation operators (or vice versa) have not been included, since they would arise only in the case of the relatively uncommon two-body operators which are antisymmetric in *both* the space *and* spin–isospin variables.] The Kronecker products $[f_1] \times [f_2]$ with $[f_2] = [211]$, [22], or [422] are not simply reducible. If $[f_1]$ is the most general irreducible representation of $SU(4)$, these products will contain the irreducible representation $[f_1]$ itself with multiplicities as high as 3, 2, or 6, respectively. For the special representations to be considered in this investigation, however, these multiplicities are never greater than 2; and in this case the nature of the operators themselves furnishes a canonical method of resolving the multiplicity problem.

3. THE SPECIAL $SU(4)$ REPRESENTATIONS; CONSTRUCTION OF STATE VECTORS

Most of the Wigner supermultiplets of actual importance in shell-model studies fall into a few special classes for which the spin and isospin quantum numbers are sufficient for a complete classification of the states of a given irreducible representation. The reduction of the irreducible representations of $SU(4)$ into the representations of $SU(2) \times SU(2)$ has been

[13] M. Hamermesh, *Group Theory and its Application to Physical Problems* (Addison-Wesley Publ. Co., Reading, Mass., 1962), Sec. 7-12.

TABLE IV. Branching formula for $[yy0] \rightarrow (S, T)$.

(S, T)						
$(y, 0)$						
$(y-1, 1)$						
$(y-2, 2)$	$(y-2, 0)$					
$(y-3, 3)$	$(y-3, 1)$					
$(y-4, 4)$	$(y-4, 2)$	$(y-4, 0)$				
.	.	.	$\cdots$	$(y-2i, 0)$		
.	.	.				
.	.	.	$\cdots$	.		
.	.	.		.		
$(3, y-3)$	$(3, y-5)$	$(3, y-7)$	$\cdots$	.	$\cdots$	
$(2, y-2)$	$(2, y-4)$	$(2, y-6)$	$\cdots$	$(2, y-2i-2)$	$\cdots$	
$(1, y-1)$	$(1, y-3)$	$(1, y-5)$	$\cdots$	$(1, y-2i-1)$	$\cdots$	
$(0, y)$	$(0, y-2)$	$(0, y-4)$	$\cdots$	$(0, y-2i)$	$\cdots$	$(0, 0)$[a]

[a] The last column has the entry (0, 0) for y = even integer; or (1, 0) and (0, 1) for y = odd integer.

TABLE V. Branching formula for $[y\,y-1\,0]$ or $[yy1] \rightarrow (S, T)$.

(S, T)						
$(y-\frac{1}{2}, \frac{1}{2})$						
$(y-\frac{3}{2}, \frac{3}{2})$	$(y-\frac{3}{2}, \frac{1}{2})$					
$(y-\frac{5}{2}, \frac{5}{2})$	$(y-\frac{5}{2}, \frac{3}{2})$	$(y-\frac{5}{2}, \frac{1}{2})$				
$(y-\frac{7}{2}, \frac{7}{2})$	$(y-\frac{7}{2}, \frac{5}{2})$	$(y-\frac{7}{2}, \frac{3}{2})$	$(y-\frac{7}{2}, \frac{1}{2})$			
.	.	.	.	.		
.	.	.	.	..		
.	.	.	.	...		
$(\frac{3}{2}, y-\frac{3}{2})$	$(\frac{3}{2}, y-\frac{5}{2})$	$(\frac{3}{2}, y-\frac{7}{2})$	$(\frac{3}{2}, y-\frac{9}{2})$	$\cdots$	$(\frac{3}{2}, \frac{1}{2})$	
$(\frac{1}{2}, y-\frac{1}{2})$	$(\frac{1}{2}, y-\frac{3}{2})$	$(\frac{1}{2}, y-\frac{5}{2})$	$(\frac{1}{2}, y-\frac{7}{2})$	$\cdots$	$(\frac{1}{2}, \frac{3}{2})$	$(\frac{1}{2}, \frac{1}{2})$

discussed in general algebraic form by Racah.[14] Racah's technique leads to the branching law giving the set of possible ST values in a given irreducible representation $[f]$, together with their multiplicities. In particular, it can be seen that these multiplicities are never greater than one in the following classes of $SU(4)$ representations:

$$[yy0]\ [y\,y-1\,0]\ [y00]\ [y10]\qquad [y11]$$
$$[yy1]\qquad [yyy]\ [yy\,y-1]\ [y\,y-1\,y-1], \tag{26}$$

where y = arbitrary integer (including zero, when possible), and where conjugate pairs of representations have been arranged in the same columns. Many-nucleon wavefunctions made up entirely of pairs coupled to an orbital angular momentum of zero (seniority zero functions) have spin–isospin wavefunctions which transform according to the self-conjugate representations $[yy0]$. States with seniority 1 have spin–isospin wavefunctions which transform according to the representations $[y\,y-1\,0]$ or $[yy1]$. These representations are therefore of special interest in the study of spin-charge independent pairing interactions.[15] The irreducible representations $[y00]$ imply totally symmetric spin–isospin wavefunctions, hence totally antisymmetric spatial wavefunctions. Such functions are therefore of interest in nuclear problems only for small values of the integer y. However, they are relatively simple and are therefore included in the present investigation.

The set of possible ST values for the irreducible representations $[yy0]$ is listed in Table IV. They are arranged in columns for which $y - S - T = 0, 2, 4, \cdots$, even integer only. The set of possible ST values for $[y\,y-1\,0]$ or $[yy1]$ is listed in Table V, where they are arranged in columns for which

$$y - S - T = 0, 1, 2, 3, \cdots;$$

that is, $y - S - T$ can be alternately even or odd. In the irreducible representation $[y00]$ or its conjugate $[yyy]$, the possible ST values are restricted to those with $T = S$, where $S = \frac{1}{2}y,\ \frac{1}{2}y - 1,\ \frac{1}{2}y - 2, \cdots$, ending in $S = 0$ (or $\frac{1}{2}$) for y = even (or odd) integer. In the representation $[y10]$ or its conjugate $[yy\,y-1]$, the possible ST values are restricted to the sets with $T = S$ or $T = S \pm 1$, starting with

$$\{ST\} = \{\tfrac{1}{2}(y+1)\,\tfrac{1}{2}(y-1)\},\ \{\tfrac{1}{2}(y-1)\,\tfrac{1}{2}(y+1)\},$$
$$\{\tfrac{1}{2}(y-1)\,\tfrac{1}{2}(y-1)\}, \cdots,$$

and ending with $\{11\}$, $\{10\}$, $\{01\}$, or $\{\frac{3}{2}\,\frac{1}{2}\}$, $\{\frac{1}{2}\,\frac{3}{2}\}$, $\{\frac{1}{2}\,\frac{1}{2}\}$, for y = odd or even integer, respectively. In the representation $[y11]$ or its conjugate $[y\,y-1\,y-1]$,

[14] G. Racah, Rev. Mod. Phys. **21**, 494 (1949).
[15] S. C. Pang, Nucl. Phys. **A128**, 497 (1969).

TABLE VI. Construction of state vectors. The overall normalization coefficients, denoted by $\mathcal{N}$, are given by the appropriate products of the normalization coefficients $N_{\alpha\beta}^{[f]}(S, T)$ given in Table VII.

$|[yy0]\{ST\}\rangle = \mathcal{N} O^q_{-1-1} O^p_{11} |[yy0]\{y0\}\rangle$; $p = \frac{1}{2}(y - S + T), q = \frac{1}{2}(y - S - T)$

$|[y\,y-1\,0]\{ST\}\rangle = \mathcal{N} O^q_{-11} O^p_{-10} |[y\,y-1\,0]\{y-\frac{1}{2}, \frac{1}{2}\}\rangle$; $p = (y - S - T), q = T - \frac{1}{2}$

$|[y00]\{ST\}\rangle = \mathcal{N} O^p_{-1-1} |[y00]\{\frac{1}{2}y, \frac{1}{2}y\}\rangle$; $p = \frac{1}{2}y - S$

$|[y10]\{ST\}\rangle = \mathcal{N} O^r_{-10} O^q_{-11} O^p_{-1-1} |[y10]\{\frac{1}{2}(y+1), \frac{1}{2}(y-1)\}\rangle$

with $p = \frac{1}{2}(y+1) - S$, $q = 0$, $r = 0$, for $ST = S, S-1$,
$p = \frac{1}{2}(y+1) - S$, $q = 0$, $r = 1$, for $ST = S-1, S-1$,
$p = \frac{1}{2}(y+1) - S$, $q = 1$, $r = 0$, for $ST = S-1, S$

$|[y11]\{ST\}\rangle = \mathcal{N} O^r_{0-1} O^q_{-10} O^p_{-1-1} |[y11]\{\frac{1}{2}y, \frac{1}{2}y\}\rangle$

with $p = \frac{1}{2}y - S$, $q = 0$, $r = 0$, for $ST = SS$,
$p = \frac{1}{2}y - S$, $q = 0$, $r = 1$, for $ST = S, S-1$,
$p = \frac{1}{2}y - S$, $q = 1$, $r = 0$, for $ST = S-1, S$

the possible ST values are also restricted by the conditions $T = S$ or $T = S \pm 1$. Now the $\{ST\}$ values start with $\{\frac{1}{2}y\,\frac{1}{2}y\}$, $\{\frac{1}{2}y\,\frac{1}{2}y-1\}$, $\{\frac{1}{2}y-1\,\frac{1}{2}y\}$, $\cdots$, but end with $\{11\}$, $\{10\}$, $\{01\}$, or $\{\frac{3}{2}\,\frac{1}{2}\}$, $\{\frac{1}{2}\,\frac{3}{2}\}$, $\{\frac{1}{2}\}$ for y = even or odd integer, respectively.

For the irreducible representations of the above types, the full set of state vectors can be constructed by a successive application of step-down operators $O_{\alpha\beta}$, defined by Eqs. (11)–(13), beginning with the operator acting on the highest-weight state: $\{ST\} = \{PP'\}$. The details of the construction for the five special classes of $SU(4)$ representations (26) are shown in Table VI. The basic numbers in these constructions are the normalization coefficients $N_{\alpha\beta}^{[f]}(S, T)$. Once these are determined, the matrix elements of the generators E_{ab} can be calculated with the aid of the relations of Tables II and III. The matrix elements of E_{ab} in turn can be taken to form the starting point for the calculation of the $SU(4)$ Wigner coefficients. The normalization coefficients needed for the construction of the state vectors for the representations (26) are given in Table VII. The details of the technique used in their calculation are illustrated by two examples in Appendix A.

State vectors $|\{ST\}\rangle$ for the representations conjugate to those included in Tables VI and VII must be constructed by exactly the same sequence of step operators. The phase factors needed to relate a state vector to its conjugate are thus determined by the integers p, q, r defined in Table VI. It is convenient to define the conjugation operator K:

$$|[f]SM_S, TM_T\rangle^* \equiv K\,|[f]SM_S, TM_T\rangle, \quad (27)$$

where $KcK^{-1} = c^*$ (c = complex number). When applied to the infinitesimal operators, the conjugation operator has the transformation properties

$$KJ_{ij}K^{-1} = -J_{ij}, \quad KE_{ab}K^{-1} = -E_{-a-b},$$
$$KS_aK^{-1} = -S_{-a}, \quad KT_aK^{-1} = -T_{-a}.$$

From these properties and the relations of Tables II and III, it follows that

$$\begin{aligned} KO_{\alpha\beta}\,|[f]\{ST\}\rangle &= (-1)^{1+\eta([f],S,T)} \frac{2^{S+\alpha+T+\beta}}{(2(S+\alpha))!\,(2(T+\beta))!} \\ &\quad \times S_-^{2(S+\alpha)} T_-^{2(T+\beta)} O_{\alpha\beta}\,|[f^*]\{ST\}\rangle \\ &= (-1)^{1+\eta([f],S,T)} N_{\alpha\beta}^{[f]}(S, T)\,|[f^*] \\ &\quad \times (S+\alpha, M_S = -S-\alpha) \\ &\quad \times (T+\beta, M_T = -T-\beta)\rangle, \end{aligned} \quad (28)$$

where the conjugation phase factor $\eta([f], S, T)$ is defined by Eq. (19). From Eq. (28) it can be seen that

$$\eta([f], S, T) = \eta([f], S = P, T = P') + p + q + r, \quad (29)$$

where the phase factor for the highest-weight state $\{S = P, T = P'\}$ can be chosen quite arbitrarily. In this investigation we have made our choice such that the single-nucleon creation and annihilation operators as well as the operators **S** and **T** have conjugation properties standard for ordinary spherical tensor operators, Eqs. (20) and (21). These requirements are satisfied by setting $\eta([f], P, P') = 0$ for all representations except $[y11]$. In this case it is convenient to set $\eta([y11], \frac{1}{2}y, \frac{1}{2}y) = -(y+1)$. Results giving the full (y, S, T)-dependence of the phase factors are collected in Table VIII.

It should be pointed out that, besides the general y dependence, there is an additional arbitrariness in the phase factor η in those irreducible representations in which $y - S - T$ can take on both even and odd values. In the representation $[y\,y-1\,0]$, for example, states with $y - S - T$ = odd integer are constructed from neighboring states with $y - S - T$ = even by means of the step operator O_{-10}, in the prescription of Table VI. According to Eq. (28), the single-

TABLE VII. The normalization factors.

$SU(4)$ representation	$N_{\alpha\beta}(S, T)$	Algebraic factor	
$[yy0]$	$N_{-1-1}(S, T)$	$= \left[\frac{ST(y+2-S-T)(y+2+S+T)}{(2S+1)(2T+1)}\right]^{\frac{1}{2}}$	
	$N_{-11}(S, T)$	$= \left[\frac{S(T+1)(y+3-S+T)(y+1+S-T)}{(2S+1)(2T+3)}\right]^{\frac{1}{2}}$	
$[y\,y-1\,0]$	$N_{-10}(S, T)$	$= \left[\frac{(2S-1)(y+2-S+T)(y+2+S+T)}{16S(T+1)^2}\right]^{\frac{1}{2}}$	for $(-1)^{y-S-T}=+1$
		$= \left[\frac{(2S-1)(y+1-S-T)(y+1+S-T)}{16S(T+1)^2}\right]^{\frac{1}{2}}$	for $(-1)^{y-S-T}=-1$
	$N_{-11}(S, T)$	$= \left[\frac{(2S-1)(2T+1)(y+S-T)(y+2-S+T)}{16S(T+1)}\right]^{\frac{1}{2}}$	for $(-1)^{y-S-T}=+1$
		$= \left[\frac{(2S-1)(2T+1)(y+1+S-T)(y+3-S+T)}{16S(T+1)}\right]^{\frac{1}{2}}$	for $(-1)^{y-S-T}=-1$
$[y00]$	$N_{-1-1}(S, S)$	$= \left[\frac{(2S-1)(y+2-2S)(y+2+2S)}{4(2S+1)}\right]^{\frac{1}{2}}$	
$[y10]$	$N_{-1-1}(S, S-1)$	$= \left[\frac{(2S-3)(y+3-2S)(y+1+2S)}{4(2S-1)}\right]^{\frac{1}{2}}$	
	$N_{-11}(S, S-1)$	$= \frac{\{y+1+4S^2\}}{2S(S+1)}$	
	$N_{-10}(S, S-1)$	$= \frac{1}{2S}\left[\frac{(S-1)(y+1+2S)(y+1)}{S}\right]^{\frac{1}{2}}$	
$[y11]$	$N_{-1-1}(S, S)$	$= \left[\frac{(S-1)(S+1)(2S-1)(y+2-2S)(y+2+2S)}{4S^2(2S+1)}\right]^{\frac{1}{2}}$	
	$N_{-10}(S, S) = N_{0-1}(S, S)$	$= \left[\frac{(2S-1)(y+2+2S)(y+2)}{4S(S+1)(2S+1)}\right]^{\frac{1}{2}}$	

step operation O_{-10} implies a change in the phase $(-1)^\eta$. It would, of course, have been possible to construct the states with $y-S-T=$ odd from the even neighbors by means of the operator $O_{0-1}O_{-11}$ instead. This double-step operation would have implied no change in the phase $(-1)^\eta$. However, this arbitrariness in the phase factor η is no more bothersome than the arbitrariness of its y dependence. States with $y-S-T=$ even or odd fall into two distinct families. It will be seen that the algebraic structure of the $SU(4)$ Wigner coefficients is different for the two types of states and will depend on the parity of $y-S-T$. Since states with $y-S-T=$ even or odd must be treated separately, it is not surprising that their relative phase behavior under conjugation may be arbitrary. In this investigation, the choice of phase factors is that implied by the constructions of Table VI; the resultant phase factors to be used are those shown in Table VIII.

The irreducible tensor operators of greatest interest in the applications to nuclear problems transform according to the representations [1], [1³], [2], [2³], [1²], [211], [22], and [422] (Sec. 2.8). All but [422] are special cases of one of the representations enumerated in (26), so that their components are completely labeled by the spin–isospin quantum numbers. The reduction of the 84-dimensional representation [422] into representations of $SU(2)\times SU(2)$ leads to the following set of possible $\{ST\}$ values:

$$\begin{array}{lll}\{22\} & \{21\} & \{20\}\\ \{12\} & \{11\}^2 & \\ \{02\} & & \{00\}.\end{array}$$

TABLE VIII. Conjugation phase factors.

$[f]$	$(-1)^\eta$
$[yy0]$	$(-1)^{y-S}=(-1)^T$
$[y\,y-1\,0]$	$(-1)^{y-\frac{1}{2}-S}$
$[y00]$	$(-1)^{\frac{1}{2}y-S}$
$[y10]$	$(-1)^{\frac{1}{2}(y+1)-S}$
$[y11]$	$(-1)^{\frac{1}{2}y+1+\min(S,T)}$
$[422]$	$(-1)^{S+T+\mu(1,1)^a}$

[a] $\mu(1,1)=\mu\delta_{S1}\delta_{T1}$, where $\mu=0$ for the state $|\{11\}s\rangle$, $\mu=1$ for the state $|\{11\}a\rangle$.

TABLE IX. Normalized state vectors for [422]. The state vectors $|[422]\, SM_S = S,\ TM_T = T\rangle$ are abbreviated by $|\{ST\}\rangle$.

$\|\{21\}\rangle = (1/\sqrt{2})O_{0-1}\|\{22\}\rangle;$	$\|\{12\}\rangle = (1/\sqrt{2})O_{-10}\|\{22\}\rangle$
$\|\{20\}\rangle = (\sqrt{3}/4)(O_{0-1})^2\|\{22\}\rangle;$	$\|\{02\}\rangle = (\sqrt{3}/4)(O_{-10})^2\|\{22\}\rangle$
$\|\{11\}a\rangle = (1/\sqrt{2})O_{-1-1}\|\{22\}\rangle;$	$\|\{11\}s\rangle = (1/\sqrt{3})O_{0-1}O_{-10}\|\{22\}\rangle$
$\|\{00\}\rangle = (3/2\sqrt{10})(O_{-1-1})^2\|\{22\}\rangle$	

There are two independent states with $\{ST\} = \{11\}$. The most natural way of constructing the full set of states $|\{ST\}\rangle$ by means of step-down operators acting on the highest-weight state $|\{22\}\rangle$ is shown in Table IX. States $|\{ST\}\rangle$ of this self-conjugate representation constructed by means of an even (or odd) number of step-down operations are symmetric (or antisymmetric), respectively, under conjugation. This gives a natural way of distinguishing the two independent states with $\{ST\} = \{11\}$. The state constructed by means of the single-step operator O_{-1-1} is antisymmetric, while the state constructed by means of the double-step operator $O_{0-1}O_{-10}$ is symmetric under conjugation. These two states, denoted by $|\{11\}a\rangle$ and $|\{11\}s\rangle$, respectively, are automatically orthogonal to each other. The symmetry label under conjugation thus forms a natural choice for the needed additional quantum number. It is interesting to note that neither of these states is an eigenvector of the operators Ω and Φ of Eq. (7).

4. $SU(4)$ WIGNER AND RACAH COEFFICIENTS

4.1. Definitions: Orthonormality

The $SU(4)$ Wigner coefficients are the elements of the matrix which reduces the Kronecker product of two irreducible representations of $SU(4)$. They are defined by

$$\begin{aligned}|([f^{(1)}][f^{(2)}])[f]\rho;\, \omega\varphi,\, SM_S TM_T\rangle \\ = \sum_{\substack{\omega_1\varphi_1 S_1 M_{S_1} T_1 M_{T_1} \\ \omega_2\varphi_2 S_2 M_{S_2} T_2 M_{T_2}}} |[f^{(1)}]\omega_1\varphi_1,\, S_1M_{S_1},\, T_1M_{T_1}\rangle \\ \times |[f^{(2)}]\omega_2\varphi_2,\, S_2M_{S_2},\, T_2M_{T_2}\rangle \\ \times \langle[f^{(1)}]\omega_1\varphi_1 S_1M_{S_1}T_1M_{T_1}; \\ \times [f^{(2)}]\omega_2\varphi_2 S_2M_{S_2}T_2M_{T_2}\,|\,[f]\omega\varphi SM_S TM_T\rangle_\rho. \end{aligned} \tag{30}$$

That is, the full $SU(4)$ Wigner coefficient can be considered as the scalar product of a coupled function with a product of uncoupled functions, the latter specified by the 12 quantum numbers $\omega_i\varphi_i$, $S_iM_{S_i}$, $T_iM_{T_i}$ with $i = 1$ and 2. Since a state $[f]$ may occur more than once in the product $[f^{(1)}] \times [f^{(2)}]$, the coupled state is not fully specified by the six quantum numbers $\omega\varphi$, SM_S, TM_T and the three irreducible representation labels for $[f]$. An additional label ρ is needed to distinguish between the various possible states with the same $[f]\omega\varphi$, SM_S, TM_T. (In principle, the labels ρ should be given by the eigenvalues of three additional operators. Such operators must lie outside the group $SU(4)$.[16] In practice the labels ρ are chosen through a set of canonical operators of irreducible tensor character $[f^{(2)}]$, for which only a specific reduced matrix element has a nonzero value, where these are defined in Sec. 4.2.

The full $SU(4)$ Wigner coefficient can be factored into a reduced $SU(4) \supset [SU(2) \times SU(2)]$ coefficient (to be denoted by a double bar) and two ordinary $SU(2)$ or angular momentum coupling coefficients for the spin and isospin spaces which carry the dependence on M_S and M_T:

$$\begin{aligned}\langle[f^{(1)}]\omega_1\varphi_1 S_1M_{S_1}T_1M_{T_1};\, [f^{(2)}]\omega_2\varphi_2 \\ \times S_2M_{S_2}T_2M_{T_2}\,|\,[f]\omega\varphi SM_S TM_T\rangle_\rho \\ = \langle[f^{(1)}]\omega_1\varphi_1 S_1T_1;\, [f^{(2)}]\omega_2\varphi_2 S_2T_2\,\|\,[f]\omega\varphi ST\rangle_\rho \\ \times \langle S_1M_{S_1}S_2M_{S_2}\,|\,SM_S\rangle\langle T_1M_{T_1}T_2M_{T_2}\,|\,TM_T\rangle. \end{aligned} \tag{31}$$

The reduced or double-barred coefficients can be identified with the spin–isospin factor[2,8] of the fractional parentage coefficients which describe the coupling of n_1 nucleons of spin–isospin symmetry $[f^{(1)}]$ with n_2 nucleons of spin–isospin symmetry $[f^{(2)}]$ to a state of n nucleons of spin–isospin symmetry $[f]$. [From now on the term $SU(4)$ Wigner coefficient will be used to refer to these reduced (or double-barred) coefficients.] The reduced coefficients satisfy the orthonormality relations:

for *fixed* S, T:

$$\begin{aligned}\sum_{\substack{\omega_1\varphi_1 S_1T_1 \\ \omega_2\varphi_2 S_2T_2}} \langle[f^{(1)}]\omega_1\varphi_1 S_1T_1;\, [f^{(2)}]\omega_2\varphi_2 S_2T_2\,\|\,[f]\omega\varphi ST\rangle_\rho \\ \times \langle[f^{(1)}]\omega_1\varphi_1 S_1T_1;\, [f^{(2)}]\omega_2\varphi_2 S_2T_2\,\|\,[f']\omega'\varphi' ST\rangle_{\rho'} \\ = \delta_{[f][f']}\delta_{\omega\omega'}\delta_{\varphi\varphi'}\delta_{\rho\rho'}; \end{aligned} \tag{32a}$$

[16] L. C. Biedenharn, A. Giovannini, and J. D. Louck, J. Math. Phys. **8**, 691 (1967).

and again for *fixed* S, T:

$$\sum_{[f]\rho\omega\varphi} \langle [f^{(1)}]\omega_1\varphi_1 S_1 T_1; [f^{(2)}]\omega_2\varphi_2 S_2 T_2 \parallel [f]\omega\varphi ST\rangle_\rho \times \langle [f^{(1)}]\omega_1'\varphi_1' S_1' T_1'; [f^{(2)}]\omega_2'\varphi_2' S_2' T_2' \parallel [f]\omega\varphi ST\rangle_\rho = \delta_{\omega_1\omega_1'}\delta_{\varphi_1\varphi_1'}\delta_{S_1S_1'}\delta_{T_1T_1'}\delta_{\omega_2\omega_2'}\delta_{\varphi_2\varphi_2'}\delta_{S_2S_2'}\delta_{T_2T_2'}. \quad (32b)$$

In the applications to be considered in this investigation, the representations $[f]$ are restricted to the special classes for which the quantum numbers ω and φ are not needed and will henceforth be omitted in the expressions for the $SU(4)$ Wigner coefficients. (Unless labels ω and φ are explicitly shown, it will be understood that the representation belongs to one of the special classes for which S and T are sufficient for a complete classification of states.)

4.2. Matrix Elements of Tensor Operators; Wigner–Eckart Theorem

The matrix elements of an $SU(4)$ irreducible tensor operator $T^{[f]}_{(SM_S)(TM_T)}$ can be expressed in terms of a generalized Wigner–Eckart theorem by a product of factors involving the appropriate Wigner coefficients and reduced matrix elements which are independent of the quantum numbers S, T, M_S, M_T, (ω, φ if needed):

$$\langle [f'']S''M_S''T''M_T''|\, T^{[f]}_{(SM_S)(TM_T)}\, |[f']S'M_S'T'M_T'\rangle = \sum_\rho \langle [f'']\|\, T^{[f]}\, \|[f']\rangle_\rho \times \langle [f']S'T'; [f]ST \parallel [f'']S''T''\rangle_\rho \times \langle S'M_S'SM_S \mid S''M_S''\rangle\langle T'M_T'TM_T \mid T''M_T''\rangle. \quad (33)$$

If the representation $[f'']$ occurs only once in the reduction of the product $[f'] \times [f]$, the labels ρ and summations over ρ are not needed. The Wigner–Eckart theorem then takes its usual form. If the product $[f'] \times [f]$ is not simply reducible, the Wigner–Eckart theorem, Eq. (33), can be used to define the labels by a choice of canonical operators whose reduced matrix elements have special values.

In the applications to nuclear problems (Sec. 5), the multiplicity problem arises only in connection with the Kronecker products $[f'] \times [211]$ and $[f'] \times [422]$. The labels ρ are needed only for $[f'] = [f'']$, $[f] = [211]$ or $[422]$ in Eq. (33). In these two cases there is a straightforward choice for the canonical operators used to define ρ. Since the infinitesimal operators $\mathbf{E}$ transform according to the representation $[211]$, the matrix elements of these operators can be used to define the label ρ for $[f] \times [211] \to [f]$. The appropriately normalized matrix elements of the components of $\mathbf{E}$ can be identified with the $SU(4)$ Wigner coefficients labeled with $\rho = 1$. Specifically,

$$\langle [f]\|\, \mathbf{E}\, \|[f]\rangle_\rho = 0 \quad \text{for} \quad \rho \neq 1, \quad (34a)$$

$$\langle [f]\|\, \mathbf{E}\, \|[f]\rangle_{\rho=1} = [C(SU_4)]^{\frac{1}{2}}, \quad (34b)$$

and

$$\langle [f]S''M_S''T''M_T''|\, E_{ab}\, |[f]S'M_S'T'M_T'\rangle = (-1)^{\chi(a,b)}[C(SU_4)]^{\frac{1}{2}}\langle [f]S'T'; [211]11 \parallel [f]S''T''\rangle_{\rho=1} \times \langle S'M_S'1a \mid S''M_S''\rangle\langle T'M_T'1b \mid T''M_T''\rangle, \quad (35)$$

where the phase factor $(-1)^{\chi(a,b)}$ is given by the standard phase of the particular component E_{ab}, as indicated in the last column of Table I. Coefficients with $\rho = 2$, $\langle [f]S'T'; [211]ST \parallel [f]S''T''\rangle_{\rho=2}$, are then fixed by the orthogonality (32a). [For the special $SU(4)$ representations enumerated in Sec. 3, the multiplicity is never greater than two.]

The operators E_{ab} are one-body operators, $a^\dagger a$, with irreducible tensor character $[211]$ which are complete space scalars. This suggests that the two-body operators, $a^\dagger a^\dagger aa$, with irreducible tensor character $[422]$ which are complete space scalars, can be used to define the labels ρ for the coefficients which reduce $[f] \times [422]$ into $[f]$. The $S = M_S = T = M_T = 2$ component of such an operator, for example, would have the specific form

$$\sum_{\alpha\beta} a^\dagger_{\alpha\frac{1}{2}\frac{1}{2}} a^\dagger_{\beta\frac{1}{2}\frac{1}{2}} a_{\beta-\frac{1}{2}-\frac{1}{2}} a_{\alpha-\frac{1}{2}-\frac{1}{2}}. \quad (36)$$

The appropriately normalized coefficients which give the ST dependence of the matrix elements of such operators are to be identified with the coefficients $\langle [f]S'T'; [422]ST \parallel [f]S''T''\rangle_{\rho=1}$; that is, those with $\rho = 1$. Coefficients with $\rho = 2$ can again be constructed by means of the orthogonality requirement.

4.3. Phase Convention

The over-all phase of the $SU(4)$ Wigner coefficients is arbitrary. It is fixed by a generalized Condon–Shortley phase convention. The $SU(4)$ Wigner coefficients can be chosen to be real, and the so-called leading coefficient connecting the highest-weight state $S_1T_1 = P_1P_1'$ of the representation $[f^{(1)}]$ with the highest-weight state $S_3T_3 = P_3P_3'$ of the representation $[f^{(3)}]$ is chosen to be positive. For most of the simple products $[f^{(1)}] \times [f^{(2)}] \to [f^{(3)}]$ this choice of S_1T_1, S_3T_3 uniquely determines S_2T_2. If it does not, the leading coefficient is specified by a further choice of S_2T_2 (the specific S_2T_2 values to be singled out will be denoted by a bar: $\bar{S}_2\bar{T}_2$), such that

$$\langle [f^{(1)}]P_1P_1'; [f^{(2)}]\bar{S}_2\bar{T}_2 \parallel [f^{(3)}]P_3P_3'\rangle > 0. \quad (37)$$

In the case of the coefficients in the reduction $[f] \times [211] \to [f]$, it is convenient to set $\bar{S}_2\bar{T}_2 = 10$, or

equally well 01 (rather than 11), so that the matrix elements of S_0 and T_0 have their conventional positive values. In all other cases, $\bar{S}_2\bar{T}_2$ will be chosen as the largest possible values of S_2T_2 consistent with the restriction $S_1T_1 = P_1P_1'$, $S_3T_3 = P_3P_3'$.

4.4. Symmetry Properties of the Wigner Coefficients

The symmetry properties of the $SU(4)$ Wigner coefficients may, in the most general case, be complicated by the state-labeling problem and the multiplicity problem. For those Wigner coefficients for which neither the quantum numbers ω and φ nor the labels ρ are needed, the symmetry properties can be derived by standard techniques.[17] They follow from the conjugation properties of the state vectors, Eq. (19). Combined with the well-known symmetry properties for the ordinary spin–isospin angular momentum coupling coefficients, the symmetry properties for the reduced $SU(4)$ Wigner coefficients follow from those of the full $SU(4)$ Wigner coefficients.

When *neither* ω, φ, *nor* ρ *are needed*, they are

$$\text{(I)}\ \langle[f^{(1)*}]S_1T_1;\,[f^{(2)*}]S_2T_2 \parallel [f^{(3)*}]S_3T_3\rangle = (-1)^{\eta^{(1)}+\eta^{(2)}-\eta^{(3)}}\langle[f^{(1)}]S_1T_1;\,[f^{(2)}]S_2T_2 \parallel [f^{(3)}]S_3T_3\rangle, \tag{38}$$

where the conjugation phase factors η are enumerated in Table VIII.

$$\text{(II)}\ \langle[f^{(1)}]S_1T_1;\,[f^{(2)}]S_2T_2 \parallel [f^{(3)}]S_3T_3\rangle = (-1)^{\sigma+\eta^{(2)}+S_1+S_2-S_3+T_1+T_2-T_3} \times \left[\frac{\dim[f^{(3)}](2S_1+1)(2T_1+1)}{\dim[f^{(1)}](2S_3+1)(2T_3+1)}\right]^{\frac{1}{2}} \times \langle[f^{(3)}]S_3T_3;\,[f^{(2)*}]S_2T_2 \parallel [f^{(1)}]S_1T_1\rangle, \tag{39}$$

where the over-all phase in this relation is fixed by the convention (37), giving

$$\sigma = P_1 - P_3 + P_1' - P_3' + \eta([f^{(2)}]\bar{S}_2\bar{T}_2) + \bar{S}_2 + \bar{T}_2, \tag{40}$$

and dim $[f^{(i)}]$ stands for the dimension of the irreducible representation $[f_1^{(i)}f_2^{(i)}f_3^{(i)}]$:

$$\dim[f_1f_2f_3] = \tfrac{1}{12}(f_1-f_2+1)(f_1-f_3+2) \times (f_2-f_3+1)(f_1+3)(f_2+2)(f_3+1). \tag{41}$$

A special case of relation (II) gives

$$\langle[f]ST;\,[f^*]ST \parallel [0]00\rangle = (-1)^{\sigma+\eta([f],S,T)}\left[\frac{(2S+1)(2T+1)}{\dim[f]}\right]^{\frac{1}{2}}, \tag{42}$$

where $\sigma = 0$ for all the representations enumerated in (26) (except $[y11]$ and its conjugate, for which $\sigma = y+1$). Finally, the symmetry property involving the simple interchange of representations (1) and (2) is given by

$$\text{(III)}\ \langle[f^{(1)}]S_1T_1;\,[f^{(2)}]S_2T_2 \parallel [\ ^{(3)}]S_3T_3\rangle = (-1)^{\nu+S_1+S_2-S_3+T_1+T_2-T_3} \times \langle[f^{(2)}]S_2T_2;\,[f^{(1)}]S_1T_1 \parallel [f^{(3)}]S_3T_3\rangle, \tag{43}$$

where the phase factor $(-1)^\nu$, through the convention (37), can be identified with the sign of the coefficient:

$$\langle[f^{(1)}]\bar{S}_1\bar{T}_1;\,[f^{(2)}]P_2P_2' \parallel [f^{(3)}]P_3P_3'\rangle.$$

The symmetry property (III) is not of very great interest, but the relations (I) and (II), as well as their combination, may be very useful in the applications to problems in nuclear physics and lead to a reduction in the number of coefficients which must be calculated (or tabulated).

If S and T are not sufficient to specify the states of a representation, the additional quantum numbers can always be chosen such that the symmetry relations (I)–(III) are satisfied. This requires that the state vectors have simple conjugation properties. For this purpose it may be convenient to choose quantum numbers other than ω, φ (as indicated in the case of the representation [422]). In the case of products which are not simply reducible, the symmetry relations may be dependent on the labels ρ. Only the coupling coefficients for the products $[f] \times [211] \to [f]$ and $[f] \times [422] \to [f]$ are of special interest in the applications to nuclear problems. With our choice of ρ, the symmetry relation (I) becomes

$$\text{(I)}\ \langle[f^{(1)*}]S_1T_1;\,[f^{(2)*}]S_2T_2 \parallel [f^{(3)*}]S_3T_3\rangle_\rho = (-1)^{\rho+1+\eta^{(1)}+\eta^{(2)}-\eta^{(3)}} \times \langle[f^{(1)}]S_1T_1;\,[f^{(2)}]S_2T_2 \parallel [f^{(3)}]S_3T_3\rangle_\rho, \tag{38'}$$

when $[f^{(2)}]$ is one of the self-conjugate representations [211] or [422]. The symmetry relations (II) and (III) are independent of ρ when $[f^{(2)}]$ is either of these two representations.

4.5. $SU(4)$ Racah Coefficients

The $SU(4)$ Racah coefficients are straightforward generalizations of the ordinary Racah coefficients and can be defined by a recoupling transformation for a coupled system built from the states of three irreducible representations $[f^{(i)}]$ with $i = 1, 2, 3$, and coupled to a resultant state of the representation $[f]$. Two ways of coupling such a system are illustrated in Fig. 2 by the type of diagrams introduced by French.[18]

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

[18] M. H. Macfarlane and J. B. French, Rev. Mod. Phys. 32, 567 (1960).

The recoupling process involves a unitary transformation whose matrix elements are the $SU(4)$ Racah or U coefficients:

$$|(\{([f^{(1)}][f^{(2)}])[f^{(12)}]\rho_{12}\}[f^{(3)}])[f]\rho_{12,3};\omega\varphi SM_S TM_T\rangle = \sum_{[f^{(23)}]\rho_{23}\rho_{1,23}} |([f^{(1)}]\{([f^{(2)}][f^{(3)}])[f^{(23)}]\rho_{23}\})[f]\rho_{1,23};\omega\varphi SM_S TM_T\rangle \times U([f^{(1)}][f^{(2)}][f][f^{(3)}];[f^{(12)}]\rho_{12}\rho_{12,3};[f^{(23)}]\rho_{23}\rho_{1,23}). \quad (44)$$

The U coefficients satisfy the orthogonality relations

$$\sum_{\alpha} U(\cdots;\alpha\mu)U(\cdots;\alpha\mu') = \delta_{\mu\mu'},$$
$$\sum_{\mu} U(\cdots;\alpha\mu)U(\cdots;\alpha'\mu) = \delta_{\alpha\alpha'}, \quad (45)$$

where α is a short-hand notation for $[f^{(12)}]$, ρ_{12}, $\rho_{12,3}$, and where μ is a short-hand notation for $[f^{(23)}]$, ρ_{23}, $\rho_{1,23}$. The U coefficients can be related to the $SU(4)$ Wigner coefficients by the sum

$$U([f^{(1)}][f^{(2)}][f][f^{(3)}];[f^{(12)}]\rho_{12}\rho_{12,3};[f^{(23)}]\rho_{23}\rho_{1,23}) = \sum_{\substack{\epsilon_1\epsilon_2\epsilon_3\\ \epsilon_{12}\epsilon_{23}}} \langle[f^{(1)}]\epsilon_1;[f^{(2)}]\epsilon_2 \parallel [f^{(12)}]\epsilon_{12}\rangle_{\rho_{12}}\langle[f^{(12)}]\epsilon_{12};[f^{(3)}]\epsilon_3 \parallel [f]\epsilon\rangle_{\rho_{12,3}} \times \langle[f^{(2)}]\epsilon_2;[f^{(3)}]\epsilon_3 \parallel [f^{(23)}]\epsilon_{23}\rangle_{\rho_{23}}\langle[f^{(1)}]\epsilon_1;[f^{(23)}]\epsilon_{23} \parallel [f]\epsilon\rangle_{\rho_{1,23}} U(S_1S_2SS_3;S_{12}S_{23})U(T_1T_2TT_3;T_{12}T_{23}), \quad (46)$$

where ϵ_i is a short-hand notation for S_iT_i (and $\omega_i\varphi_i$, if needed). The sums over M_{S_i} and M_{T_i} have been performed and expressed in terms of the angular momentum U coefficients (unitary or Jahn form of the S and T space Racah coefficients). The $SU(4)$ U coefficients are independent of ST, $(\omega\varphi)$, so that any convenient subgroup labeling can, in principle, be used in performing the sums over the subgroup quantum numbers. In principle, therefore, very general expressions can be given for the Racah coefficients. However, these would be unnecessarily complicated by the multiplicity labels ρ. In the actual applications, labels ρ_{12}, ρ_{23}, and $\rho_{12,3}$ are never needed; in those cases where they are needed, the label $\rho_{1,23}$ corresponds to a multiplicity of two only. The most useful equation relating the $SU(4)$ Racah and Wigner coefficients is given by

$$\sum_{\rho_{1,23}} \langle[f^{(1)}]\epsilon_1;[f^{(23)}]\epsilon_{23} \parallel [f]\epsilon\rangle_{\rho_{1,23}} U([f^{(1)}][f^{(2)}][f][f^{(3)}];[f^{(12)}]\rho_{12}\rho_{12,3};[f^{(23)}]\rho_{23}\rho_{1,23}) = \sum_{\epsilon_2\epsilon_3\epsilon_{12}} \langle[f^{(1)}]\epsilon_1;[f^{(2)}]\epsilon_2 \parallel [f^{(12)}]\epsilon_{12}\rangle_{\rho_{12}}\langle[f^{(12)}]\epsilon_{12};[f^{(3)}]\epsilon_3 \parallel [f]\epsilon\rangle_{\rho_{12,3}}\langle[f^{(2)}]\epsilon_2;[f^{(3)}]\epsilon_3 \parallel [f^{(23)}]\epsilon_{23}\rangle_{\rho_{23}} \times U(S_1S_2SS_2;S_{12}S_{23})U(T_1T_2TT_3;T_{12}T_{23}). \quad (47)$$

Except for the summation over $\rho_{1,23}$ (when needed), this is again a straightforward generalization of a relation valid for ordinary angular momentum coefficients. This equation is to be used as the basis for a buildup process whereby relatively complicated $SU(4)$ Wigner coefficients are calculated from a knowledge of very simple ones.

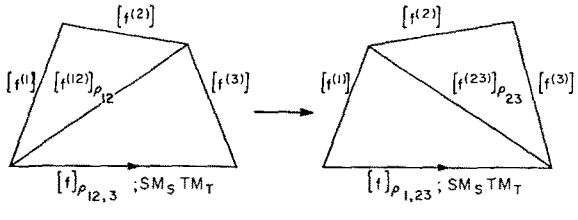


FIG. 2. Two ways of coupling states of 3 IR's to a resultant state.

Equation (47), together with Eqs. (42), (39), and (32a), also leads to the special value

$$U([f][f^{(2)}][f][f^{(2)*}];[f^{(12)}];[0]) = (-1)^{\sigma([f],[f^{(2)}],[f^{(12)}])+\sigma_2}\cdot\left[\frac{\dim[f^{(12)}]}{\dim[f]\dim[f^{(2)}]}\right]^{\frac{1}{2}}, \quad (48)$$

where $\sigma([f],[f^{(2)}],[f^{(12)}])$ is given by Eq. (40), and $\sigma_2 = 0$ unless $[f^{(2)}] = [y11]$ or its conjugate, in which case $\sigma_2 = y+1$, Eq. (42).

4.6. Method of Calculation

The calculation of the $SU(4)$ Wigner coefficients begins with the calculation of the matrix elements of the infinitesimal operators E_{ab}. These follow from

the normalization coefficients of Table VII and the relations of Tables II and III (for the details, see Appendix A and Ref. 19). The matrix elements of E_{ab} are expressed in terms of reduced $SU(4)$ Wigner coefficients by means of Eq. (35). They can be read off from the tabulations of $\langle [f]S'T'; [211]11 \,\|\, [f]S''T''\rangle_{\rho=1}$ given in Appendix B.

The simplest Wigner coefficients are those involving a coupling of $[f]$ with the one-particle representation [1] (one-particle cfp's). These can be calculated by standard recursion techniques from a knowledge of the matrix elements of the infinitesimal operators. By operating with an operator $E_{ab} = E_{ab}(1) + E_{ab}(2)$ on the state of a coupled system built from systems 1 and 2, a recursion relation for the full $SU(4)$ Wigner coefficients is obtained. For example,

$$\begin{aligned}
\sum_{S'T'} &\langle [f^{(1)}]S_1M_{S_1}T_1M_{T_1}; [1]\tfrac{1}{2}M_{S_2}\tfrac{1}{2}M_{T_2} \,|\, [f]S'(M_S+1)T'(M_T+1)\rangle \\
&\times \langle [f]S'(M_S+1)T'(M_T+1)|\, E_{11} \,|[f]SM_STM_T\rangle \\
&= \sum_{S_1'T_1'} \langle [f^{(1)}]S_1'(M_{S_1}-1)T_1'(M_{T_1}-1); [1]\tfrac{1}{2}M_{S_2}\tfrac{1}{2}M_{T_2} \,|\, [f]SM_STM_T\rangle \\
&\times \langle [f^{(1)}]S_1M_{S_1}T_1M_{T_1}|\, E_{11} \,|[f^{(1)}]S_1(M_{S_1}-1)T_1(M_{T_1}-1)\rangle \\
&+ \langle [f^{(1)}]S_1M_{S_1}T_1M_{T_1}; [1]\tfrac{1}{2}(M_{S_2}-1)\tfrac{1}{2}(M_{T_2}-1) \,|\, [f]SM_STM_T\rangle \\
&\times \langle [1]\tfrac{1}{2}M_{S_2}\tfrac{1}{2}M_{T_2}|\, E_{11} \,|[1]\tfrac{1}{2}(M_{S_2}-1)\tfrac{1}{2}(M_{T_2}-1)\rangle. \qquad (49)
\end{aligned}$$

From such recursion relations, coefficients of the above simple type have been calculated for the cases when both $[f^{(1)}]$ and $[f]$ belong to the special representations of Sec. 3. Coefficients for the coupling of $[f^{(1)}]$ with more complicated representations are then calculated by a buildup process based on the recoupling relation, Eq. (47). By setting both $[f^{(2)}]$ and $[f^{(3)}]$ equal to the one-particle representation [1] in Eq. (47), $SU(4)$ Wigner coefficients with $[f^{(23)}] = [2]$ or $[1^2]$ (two-particle cfp's) can be calculated. In this case the products $[f^{(1)}] \times [f^{(23)}]$ are simply reducible. The ρ sum in Eq. (47) is not needed, and the $SU(4)$ U coefficient serves merely as a normalization factor for the Wigner coefficients. Coefficients with $[f^{(23)}] =$ [211], [22], and [422] can be calculated through Eq. (47) by setting $[f^{(2)}]$ and $[f^{(3)}]$ equal to $[1^3]$ and [1], $[1^2]$ and $[1^2]$, and $[2^3]$ and [2], respectively. In many of these cases the multiplicity in the product $[f^{(1)}] \times [f^{(23)}]$ requires the ρ sum for the left-hand side of (47), and the simultaneous calculation of both the Wigner and U coefficients requires the solution of a simple 2×2 linear system.

Algebraic expressions for both the Wigner and Racah coefficients are tabulated in Appendix B. This appendix is preceded by a table listing the cases covered and showing the arrangement of the tables of $SU(4)$ coefficients. Wigner coefficients involving the coupling with [22] and [422] include only the coefficients needed for diagonal matrix elements of the corresponding two-body operators. The tables of Racah coefficients are also restricted to those needed for the calculation of diagonal matrix elements—that is, those with $[f^{(1)}] = [f]$, and $[f^{(2)}]$ and $[f^{(3)}]$ equal to $[1^3]$ and [1], or $[1^2]$ and $[1^2]$, and $[2^3]$ and [2], needed for the evaluation of the matrix elements of one-body, or two-body operators.

5. APPLICATIONS

The recognition that the spin–isospin part of the fractional parentage coefficients can be identified with the reduced $SU(4)$ Wigner coefficients makes it possible to perform the spin–isospin sums in the cfp expansions of nuclear matrix elements by means of the Racah formalism of Sec. 4.

The cfp's needed for the decomposition of a totally antisymmetric n-nucleon wavefunction into totally antisymmetric functions for specific sets of n_1 and n_2 nucleons can be factored into a space and a spin–isospin part[2,8]:

$$\begin{aligned}
&\langle [f^{(n_1)}]\alpha_{n_1}L_{n_1}, \beta_{n_1}S_{n_1}T_{n_1}; [f^{(n_2)}]\alpha_{n_2}L_{n_2}, \beta_{n_2}S_{n_2}T_{n_2} \,|\} \, [f^{(n)}]\alpha_nL_n, \beta_nS_nT_n\rangle \\
&\quad = \left[\frac{\mathcal{N}_{[f^{(n_1)}]}\mathcal{N}_{[f^{(n_2)}]}}{\mathcal{N}_{[f^{(n)}]}}\right]^{\frac{1}{2}} \langle [f^{(n_1)}]\alpha_{n_1}L_{n_1}; [f^{(n_2)}]\alpha_{n_2}L_{n_2} \,|\} \, [f^{(n)}]\alpha_nL_n\rangle \\
&\qquad \times \langle [f^{(n_1)}]\beta_{n_1}S_{n_1}T_{n_1}; [f^{(n_2)}]\beta_{n_2}S_{n_2}T_{n_2} \,\|\, [f^{(n)}]\beta_nS_nT_n\rangle, \qquad (50)
\end{aligned}$$

[19] S. C. Pang, "On Eight-Dimensional Quasispin," Ph.D. thesis, Univ. of Michigan, 1967.

where the spin–isospin factor has been written in the $SU(4)$ notation of Sec. 4, and where $\mathcal{N}_{[f^{(n_i)}]}$ is the dimension of the irreducible representation of the *symmetric* or *permutation* group on n_i objects described by the Young tableau $[f^{(n_i)}]$. The representation contragredient to $[f]$ under the symmetric group is denoted by $[\tilde{f}]$; that is, $[\tilde{f}]$ is obtained from $[f]$ by interchanging rows and columns in the Young tableau. (It should perhaps be pointed out that the symbol $[f]$ is usually used to denote the symmetry of the space part of the wavefunction, while $[\tilde{f}]$ is used for the spin–isospin part. In this investigation the role of the two has been interchanged for economy in writing. The tilde still implies interchange of rows and columns of the Young tableau.) The full set of space quantum numbers other than L is abbreviated by the label α; quantum numbers such as ω, φ are replaced by β. [If needed, it will be understood that these quantum numbers will be chosen such that the $SU(4)$ Wigner coefficients satisfy the symmetry relations (I)–(III).] Matrix elements of one- and two-body operators can be expressed in terms of these cfp's by the usual expansions.

5.1. One-Body Operators

It will be assumed that the one-body operator

$$\mathcal{O} = \sum_{i=1}^{n} o_i = \sum_{\alpha' \cdots m_t} \langle \alpha' l' m_l' m_s' m_t' | \, o \, | \alpha l m_l m_s m_t \rangle \, a^{\dagger}_{\alpha' l' m_l' m_s' m_t'} a_{\alpha l m_l m_s m_t} \tag{51}$$

has a definite $SU(4)$ irreducible tensor character $[f_{\mathrm{op}}]$ with components $(\mathcal{S}\mathcal{M}_{\mathcal{S}}\mathcal{T}\mathcal{M}_{\mathcal{T}})$, and spherical tensor character $\mathfrak{L}$ with component $\mathcal{M}_{\mathfrak{L}}$. The matrix element of the one-particle operator can then be factored:

$$\langle \alpha' l' m_l' m_s' m_t' | \, o \, | \alpha l m_l m_s m_t \rangle = \langle \alpha' l' \| \, o \, \| \alpha l \rangle \, \langle [1]\tfrac{1}{2}\tfrac{1}{2}; [f_{\mathrm{op}}]\mathcal{S}\mathcal{T} \, \| \, [1]\tfrac{1}{2}\tfrac{1}{2} \rangle \times \langle \tfrac{1}{2} m_s \mathcal{S}\mathcal{M}_{\mathcal{S}} \, | \, \tfrac{1}{2} m_s' \rangle \langle \tfrac{1}{2} m_t \mathcal{T}\mathcal{M}_{\mathcal{T}} \, | \, \tfrac{1}{2} m_t' \rangle \langle l m_l \mathfrak{L}\mathcal{M}_{\mathfrak{L}} \, | \, l' m_l' \rangle. \tag{52}$$

The matrix element of the one-body operator between n-nucleon states can be expressed by the cfp expansion

$$\langle [f']\alpha' L' M_L', \beta' S' M_S' T' M_T' | \, \mathcal{O} \, | [f]\alpha L M_L, \beta S M_S T M_T \rangle = n \sum_{[f^{(n-1)}]} \frac{\mathcal{N}_{[f^{(n-1)}]}}{[\mathcal{N}_{[f]}\mathcal{N}_{[f']}]^{\frac{1}{2}}} \mathcal{F}(\mathrm{space})\mathcal{F}(SU_4), \tag{53}$$

where $\mathcal{F}(\mathrm{space})$ and $\mathcal{F}(SU_4)$ are the space and spin–isospin parts of the cfp expansion which are given by

$$\mathcal{F}(\mathrm{space}) = \sum_{\substack{\alpha_{n-1} L_{n-1} \\ \alpha_1 \alpha_1' l l'}} \langle [\tilde{f}^{(n-1)}]\alpha_{n-1} L_{n-1}; [1]\alpha_1 l \, | \} \, [\tilde{f}]\alpha L \rangle \langle [\tilde{f}^{(n-1)}]\alpha_{n-1} L_{n-1}; [1]\alpha_1' l' \, | \} \, [\tilde{f}']\alpha' L' \rangle \times \langle \alpha_1' l' \| \, o \, \| \alpha_1 l \rangle \left[\frac{(2L+1)(2l'+1)}{(2L_{n-1}+1)(2\mathfrak{L}+1)} \right]^{\frac{1}{2}} (-1)^{\mathfrak{L}+L_{n-1}-l'-L} U(L l L' l'; L_{n-1}\mathfrak{L}) \langle L M_L \mathfrak{L}\mathcal{M}_{\mathfrak{L}} \, | \, L' M_L' \rangle \tag{54}$$

and

$$\mathcal{F}(SU_4) = \sum_{\beta_{n-1} S_{n-1} T_{n-1}} \langle [f^{(n-1)}]\beta_{n-1} S_{n-1} T_{n-1}; [1]\tfrac{1}{2}\tfrac{1}{2} \, \| \, [f]\beta S T \rangle \times \langle [f^{(n-1)}]\beta_{n-1} S_{n-1} T_{n-1}; [1]\tfrac{1}{2}\tfrac{1}{2} \, \| \, [f']\beta' S' T' \rangle \langle [1]\tfrac{1}{2}\tfrac{1}{2}; [f_{\mathrm{op}}]\mathcal{S}\mathcal{T} \, \| \, [1]\tfrac{1}{2}\tfrac{1}{2} \rangle \times \left[\frac{(2S+1)2}{(2S_{n-1}+1)(2\mathcal{S}+1)} \right]^{\frac{1}{2}} (-1)^{\mathcal{S}+S_{n-1}-\frac{1}{2}-S} U(S\tfrac{1}{2}S'\tfrac{1}{2}; S_{n-1}\mathcal{S}) \langle S M_S \mathcal{S}\mathcal{M}_{\mathcal{S}} \, | \, S' M_S' \rangle \times \left[\frac{(2T+1)2}{(2T_{n-1}+1)(2\mathcal{T}+1)} \right]^{\frac{1}{2}} (-1)^{\mathcal{T}+T_{n-1}-\frac{1}{2}-T} U(T\tfrac{1}{2}T'\tfrac{1}{2}; T_{n-1}\mathcal{T}) \langle T M_T \mathcal{T}\mathcal{M}_{\mathcal{T}} \, | \, T' M_T' \rangle. \tag{55}$$

With the aid of the symmetry relations (I)–(III) for the $SU(4)$ Wigner coefficients, the latter can be written

$$\mathcal{F}(SU_4) = \left\{ (-1)^{\sigma([f^{(n-1)}],[1],[f])} \left[\frac{\dim [1] \dim [f]}{\dim [f^{(n-1)}]} \right]^{\frac{1}{2}} \right\} \frac{(-1)^{\sigma_{\mathrm{op}}}}{[\dim [f_{\mathrm{op}}]]^{\frac{1}{2}}} \langle S M_S \mathcal{S}\mathcal{M}_{\mathcal{S}} \, | \, S' M_S' \rangle \langle T M_T \mathcal{T}\mathcal{M}_{\mathcal{T}} \, | \, T' M_T' \rangle \times \sum_{\beta_{n-1} S_{n-1} T_{n-1}} \langle [f]\beta S T; [1^3]\tfrac{1}{2}\tfrac{1}{2} \, \| \, [f^{(n-1)}]\beta_{n-1} S_{n-1} T_{n-1} \rangle \langle [f^{(n-1)}]\beta_{n-1} S_{n-1} T_{n-1}; [1]\tfrac{1}{2}\tfrac{1}{2} \, \| \, [f']\beta' S' T' \rangle \times \langle [1^3]\tfrac{1}{2}\tfrac{1}{2}; [1]\tfrac{1}{2}\tfrac{1}{2} \, \| \, [f_{\mathrm{op}}]\mathcal{S}\mathcal{T} \rangle U(S\tfrac{1}{2}S'\tfrac{1}{2}; S_{n-1}\mathcal{S}) U(T\tfrac{1}{2}T'\tfrac{1}{2}; T_{n-1}\mathcal{T}), \tag{56}$$

where $\sigma_{\mathrm{op}} = \delta_{[f_{\mathrm{op}}][211]}$; that is, $(-1)^{\sigma_{\mathrm{op}}} = -1$ for $[f_{\mathrm{op}}] = [211]$, $(-1)^{\sigma_{\mathrm{op}}} = +1$ for $[f_{\mathrm{op}}] = [0]$.

The coefficients in the spin–isospin sum of the last factor are now in a form in which they can be summed by means of Eq. (47). Although the first factor (enclosed by curly brackets) is made up solely of trivial dimensional and phase factors, it is convenient to write it in terms of the $SU(4)$ Racah coefficient with

$[f^{(23)}] = [0]$, Eq. (48). This makes it possible to express the resultant of the spin–isospin sum in the cfp expansion in terms of ratios of $SU(4)$ U coefficients which are independent of the particular phase conventions [such as (37)] chosen for the $SU(4)$ coefficients. The resultant expression is

$$\mathcal{F}(SU_4) = \frac{(-1)^{\delta[f_{\rm op}][211]}}{[\dim [f_{\rm op}]]^{\frac{1}{2}}} \sum_{\rho} \frac{U([f][1^3][f'][1]; [f^{(n-1)}]; [f_{\rm op}]\rho)}{U([f][1^3][f][1]; [f^{(n-1)}]; [0])} \times \langle [f]\beta ST; [f_{\rm op}]\mathcal{SC} \parallel [f']\beta' S'T' \rangle_{\rho} \langle SM_S \mathcal{SM}_{\mathcal{S}} \mid S'M'_S \rangle \langle TM_T \mathcal{CM}_{\mathcal{C}} \mid T'M'_T \rangle. \quad (57)$$

The $SU(4)$ Wigner and Racah coefficients needed for the evaluation of this expression are given in Tables A.4 and A.7 of Appendix B. If the one-body operator is a *complete* space scalar (if the reduced matrix elements of o are independent of α and l), the sum over the spatial quantum numbers is trivial, and the full matrix element has the simple form

$$\langle [f']\alpha' L' M_L, \beta' S' M'_S T' M'_T | \, O^{[f_{\rm op}],\text{space-scalar}}_{(\mathcal{SM}_{\mathcal{S}})(\mathcal{CM}_{\mathcal{C}})} \, | [f]\alpha L M_L, \beta S M_S T M_T \rangle$$
$$= \delta_{[f][f']} \delta_{\alpha\alpha'} \delta_{LL'} \langle [1] \| \, o^{[f]\rm op} \, \| [1] \rangle \frac{(-1)^{\delta[f_{\rm op}][211]}}{[\dim [f_{\rm op}]]^{\frac{1}{2}}} n \sum_{[f^{(n-1)}]} \frac{\mathcal{N}_{[f^{(n-1)}]}}{\mathcal{N}_{[f]}} \sum_{\rho} \frac{U([f][1^3][f][1]; [f^{(n-1)}]; [f_{\rm op}]\rho)}{U([f][1^3][f][1]; [f^{(n-1)}]; [0])}$$
$$\times \langle [f]\beta ST; [f_{\rm op}]\mathcal{SC} \parallel [f]\beta' S'T' \rangle_{\rho} \langle SM_S \mathcal{SM}_{\mathcal{S}} \mid S'M'_S \rangle \langle TM_T \mathcal{CM}_{\mathcal{C}} \mid T'M'_T \rangle. \quad (58)$$

The only nontrivial case involves operators of $SU(4)$ tensor character [211]. In this case the sums over the possible $(n-1)$-particle symmetries have the very simple value

$$n \sum_{[f^{(n-1)}]} \frac{\mathcal{N}_{[f^{(n-1)}]}}{\mathcal{N}_{[f]}} \frac{U([f][1^3][f][1]; [f^{(n-1)}]; [211]\rho)}{U([f][1^3][f][1]; [f^{(n-1)}]; [0])}$$
$$= 0 \quad \text{for} \quad \rho \neq 1,$$
$$= -2[C(SU_4)]^{\frac{1}{2}} \quad \text{for} \quad \rho = 1, \quad (59)$$

where the Casimir invariant $C(SU_4)$ is given by Eq. (23). The S, T-dependence of the matrix element of a space-scalar one-body operator of $SU(4)$ tensor character [211] is thus given by the single $SU(4)$ Wigner coefficient with $\rho = 1$, that is, by the matrix element of the corresponding infinitesimal operator. The only nontrivial operators of this type are the infinitesimal generators **E**, Eq. (3), which give the Gamow–Teller matrix elements in beta decay. The tables of Appendix B can thus be used to read off Gamow–Teller matrix elements for a wide class of Wigner supermultiplets.

5.2. Particle–Hole Interaction; Space-Scalar Approximation

It has been shown that a space-scalar approximation to the particle–hole interaction may give a good estimate of the full particle–hole interaction energy in nuclei near the beginning of the $2s$, $1d$ shell.[10] The matrix elements of such an interaction can be written down at once in terms of the results of Eqs. (58) and (59) for particle–hole configurations described by the weak-coupling model. In the space-scalar approximation the particle–hole interaction can be represented by

$$V_{ph} = \sum_{i,j} (-a_{00} + a_{01} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j + a_{10} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + a_{11} (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)), \quad (60)$$

where $a_{\mathcal{SC}}$ are constants, and where the summation indices i and j refer to nucleons in different major shells such as the $1p$ and $2s$, $1d$ shell. Zamick[20] has pointed out that the first two terms of Eq. (60) may be used to give a rough idea of the location of the particle–hole states. The matrix elements of the first three terms of Eq. (60) can be calculated by ordinary angular-momentum calculus. The last term is more complicated. Moreover, it may lead to important contributions to the particle–hole interaction energy in many cases.[10] It may give rise not only to important J-dependent contributions to the diagonal matrix element of the interaction, but may also give an estimate of the often significant mixing of particle–hole states with the same space structure but with different spin–isospin quantum numbers for the particle and hole configurations. The last three terms of Eq. (60) are built from space-scalar one-body operators for each shell. Each has $SU(4)$ tensor character [211] with $\mathcal{SC}$ components of 01, 10, and 11, respectively. The full tensor character of each is of the form

$$a_{\mathcal{SC}} (O^{[211]}_{\mathcal{SC}} \cdot \cdot \, O^{[211]}_{\mathcal{SC}}), \quad (61)$$

where the double dot refers to the scalar product in $\mathcal{S}$ and $\mathcal{C}$ space. It is assumed that the particle–hole state can be described in the weak-coupling model in which the Wigner supermultiplet quantum numbers for both the particle and hole configurations are good

[20] L. Zamick, Phys. Letters **19**, 580 (1965).

quantum numbers, to be denoted by $[f_p]$ and $[f_h]$, respectively. If the number of particles and holes are denoted by n_p and n_h, we shall take $[f_p]$ and $[f_h]$ to be Young tableaux describing the symmetry of the spin–isospin functions for n_p and $(N - n_h)$ nucleons, respectively, where N = number of nucleons in the closed shell. The basic form of the wavefunction is chosen to be

$$|([f_h]\alpha_h L_h S_h J_h T_h,\ [f_p]\alpha_p L_p S_p J_p T_p) J M_J T M_T\rangle, \quad (62)$$

where the subscripts p and h refer to the particle and hole configurations. In the weak-coupling description there is no further coupling of the supermultiplets $[f_p]$, $[f_h]$; but the angular momenta and isospins of the particle and hole configurations are coupled to total angular momentum J and total isospin T. Matrix elements of the operators (61) follow from Eqs. (58) and (59) {with $\langle[1]\|\mathcal{O}^{[211]}\|[1]\rangle = (15)^{\frac{1}{2}}$}, leading to

$$\begin{aligned}
&\langle([f_h]\alpha_h L_h S'_h J'_h T'_h,\ [f_p]\alpha_p L_p S'_p J'_p T'_p) J M_J T M_T|\ a_{\mathcal{ST}} \mathcal{O}^{[211]}_{\mathcal{ST}} \cdots \mathcal{O}^{[211]}_{\mathcal{ST}}\ |([f_h]\alpha_h L_h S_h J_h T_h,\ [f_p]\alpha_p L_p S_p J_p T_p) J M_J T M_T\rangle \\
&\quad = a_{\mathcal{ST}} (-1)^{J+J_h+J_{p'}} \begin{Bmatrix} J_h & J_p & J \\ J'_p & J'_h & \mathcal{S} \end{Bmatrix} (-1)^{T+T_h+T_{p'}} \begin{Bmatrix} T_h & T_p & T \\ T'_p & T'_h & \mathcal{T} \end{Bmatrix} \\
&\qquad \times [(2J_h+1)(2J'_h+1)(2J_p+1)(2J'_p+1)]^{\frac{1}{2}} (-1)^{J_{h'}+S_h+L_h+\mathcal{S}} \begin{Bmatrix} S_h & J_h & L_h \\ J'_h & S'_h & \mathcal{S} \end{Bmatrix} (-1)^{J_{p'}+S_p+L_p+\mathcal{S}} \begin{Bmatrix} S_p & J_p & L_p \\ J'_p & S'_p & \mathcal{S} \end{Bmatrix} \\
&\qquad \times [(2S'_p+1)(2T'_p+1)]^{\frac{1}{2}} 2[C(SU_4)_p]^{\frac{1}{2}} \langle [f_p] S_p T_p;\ [211]\mathcal{ST} \parallel [f_p] S'_p T'_p\rangle_{\rho=1} \\
&\qquad \times [(2S'_h+1)(2T'_h+1)]^{\frac{1}{2}} 2[C(SU_4)_h]^{\frac{1}{2}} \langle [f_h] S_h T_h;\ [211]\mathcal{ST} \parallel [f_h] S'_h T'_h\rangle_{\rho=1}, \qquad (63)
\end{aligned}$$

where it is convenient to express the ordinary angular-momentum Racah coefficients in their 6-j symbol form. The $SU(4)$ Wigner coefficients for the operators with $\mathcal{ST} = 10$, 01 are given by the simple matrix elements of $\mathbf{S}$ and $\mathbf{T}$, and have the values

$$\begin{aligned}
&[C(SU_4)]^{\frac{1}{2}} \langle [f] S T;\ [211]10 \parallel [f] S' T'\rangle_{\rho=1} \\
&\qquad = \delta_{SS'} \delta_{TT'} [S(S+1)]^{\frac{1}{2}}, \\
&[C(SU_4)]^{\frac{1}{2}} \langle [f] S T;\ [211]01 \parallel [f] S' T'\rangle_{\rho=1} \\
&\qquad = \delta_{SS'} \delta_{TT'} [T(T+1)]^{\frac{1}{2}}. \qquad (64)
\end{aligned}$$

In these two cases, therefore, Eq. (63) reduces to a simple result of ordinary angular-momentum calculus. The diagonal-matrix elements of the full interaction (60) have been given in Ref. 10. The operator with $\mathcal{ST} = 11$ can give important contributions to both the diagonal and off-diagonal matrix elements. From the symmetry relation (38′), however, it can be seen that matrix elements with $S' = S$, $T' = T$ are zero for all self-conjugate representations such as $[yy0]$ or $[211]$. For configurations with an even number of particles (or holes) the most important symmetries for the spin–isospin functions are likely to be those belonging to $SU(4)$ representations such as [0], [11], [22], $\cdots$, or [211], for which the diagonal-matrix element (63) is zero. The last term of (60) is therefore important mainly for configurations with an odd number of both particles and holes. It can, however, lead to matrix elements off-diagonal in both S_pT_p and S_hT_h for all $SU(4)$ representations, and the last term of (60) may be a major contributor to the mixing of different particle–hole states with the same space structure. The $SU(4)$ Wigner coefficients needed for the evaluation of (63) are given in Tables 4.1–4.6 of Appendix B.

5.3. Two-Body Operators

The techniques used in Sec. 5.1 can also be used to simplify the expressions for the matrix elements of a two-body operator, such as the two-body interaction

$$H = \sum_{i<j} h_{ij}. \qquad (65)$$

Such operators can be decomposed into their $SU(4)$ irreducible-tensor parts with components $(\mathcal{SM}_\mathcal{S})(\mathcal{TM}_\mathcal{T})$ and spherical-tensor character $\mathfrak{L}$ (for orbital space) with components $\mathcal{M}_\mathfrak{L}$. To be invariant under rotations in ordinary three-dimensional space such operators must be of the form

$$H^{[f_{op}]}_{\mathcal{S};\mathcal{TM}_\mathcal{T}} = \sum_{\mathcal{M}_\mathcal{S}} (-1)^{\mathcal{M}_\mathcal{S}} H^{[f_{op}];\mathfrak{L}=\mathcal{S}}_{(\mathcal{SM}_\mathcal{S})(\mathcal{TM}_\mathcal{T});\mathcal{M}_\mathfrak{L}=-\mathcal{M}_\mathcal{S}}. \quad (66)$$

The reduced matrix elements of the two-particle operators are defined by the relation

$$\begin{aligned}
&\langle [f^{(2)}]\alpha'_2 L'_2 M'_{L_2} S'_2 M'_{S_2} T'_2 M'_{T_2}|\ h^{[f_{op}];\mathfrak{L}}_{(\mathcal{SM}_\mathcal{S})(\mathcal{TM}_\mathcal{T});\mathcal{M}_\mathfrak{L}}\ |[f^{(2)}]\alpha_2 L_2 M_{L_2} S_2 M_{S_2} T_2 M_{T_2}\rangle \\
&\qquad = \langle [f^{(2)}]\alpha'_2 L'_2 \|\ h^{[f_{op}];\mathfrak{L}}\ \|[f^{(2)}]\alpha_2 L_2\rangle \langle [f^{(2)}] S_2 T_2;\ [f_{op}]\mathcal{ST} \parallel [f^{(2)}] S'_2 T'_2\rangle \\
&\qquad\quad \times \langle S_2 M_{S_2} \mathcal{SM}_\mathcal{S} \mid S'_2 M'_{S_2}\rangle \langle T_2 M_{T_2} \mathcal{TM}_\mathcal{T} \mid T'_2 M'_{T_2}\rangle \langle L_2 M_{L_2} \mathfrak{L} \mathcal{M}_\mathcal{S} \mid L'_2 M'_{L_2}\rangle. \qquad (67)
\end{aligned}$$

(For simplicity, operators antisymmetric in *both* the space and spin–isospin variables will be excluded so that the two-particle matrix elements to be considered will be restricted to those with $[f^{(2)\prime}] = [f^{(2)}]$.) The spin–isospin sums in the cfp expansion for the matrix elements of such operators can be carried out by

techniques similar to those of Sec. 5.1. The matrix element between n-nucleon states can then be given by the expression

$$\langle [f']\alpha'\beta'L'S'JM_JT'M'_T|\, H^{[f_{\rm op}]}_{\mathcal{S};\mathcal{C}\mathcal{M}_\mathcal{C}}\,|[f]\alpha\beta LSJM_JTM_T\rangle$$

$$= \tfrac{1}{2}n(n-1)\sum_{[f^{(n-2)}][f^{(2)}]}\frac{\mathcal{N}_{[f^{(n-2)}]}}{[\mathcal{N}_{[f]}\mathcal{N}_{[f']}]^{\frac{1}{2}}}\sum_{\substack{\alpha_{n-2}L_{n-2}\\ \alpha_2L_2\\ \alpha_2'L_2'}}\frac{\langle [f^{(2)}]\alpha_2'L_2'\|\, h^{[f_{\rm op}];\mathcal{S}}\,\|[f^{(2)}]\alpha_2L_2\rangle}{[\dim [f_{\rm op}]]^{\frac{1}{2}}}$$

$$\times \langle [\tilde f^{(n-2)}]\alpha_{n-2}L_{n-2};\,[\tilde f^{(2)}]\alpha_2L_2\,|\}\,[\tilde f]\alpha L\rangle\langle [\tilde f^{(n-2)}]\alpha_{n-2}L_{n-2};\,[\tilde f^{(2)}]\alpha_2'L_2'\,|\}\,[\tilde f']\alpha'L'\rangle$$

$$\times (-1)^{L_{n-2}+L_2+L+\mathcal{S}+L'+S'+J}[(2L+1)(2L_2'+1)(2S'+1)(2L'+1)]^{\frac{1}{2}}\begin{Bmatrix} L & L_2 & L_{n-2}\\ L_2' & L' & \mathcal{S}\end{Bmatrix}\begin{Bmatrix} L & S & J\\ S' & L' & \mathcal{S}\end{Bmatrix}$$

$$\times \sum_\rho \frac{U([f][f^{(2)*}][f'][f^{(2)}];\,[f^{(n-2)}];\,[f_{\rm op}]\rho)}{U([f][f^{(2)*}][f][f^{(2)}];\,[f^{(n-2)}];\,[0])}\langle [f]\beta ST;\,[f_{\rm op}]\mathcal{S}\mathcal{C}\,\|\,[f']\beta'S'T'\rangle_\rho\langle TM_T\mathcal{C}\mathcal{M}_\mathcal{C}\,|\,T'M'_T\rangle. \quad (68)$$

If the two-body operator is a *complete* space scalar (that is, if the reduced matrix elements are independent of α_2 and L_2 and if $\mathcal{L} = \mathcal{S} = 0$), the matrix element again has a very simple form which can be evaluated completely with the aid of the tabulations of $SU(4)$ Wigner and Racah coefficients of Appendix B:

$$\langle [f']\alpha'\beta'L'S'JM_JT'M'_T|\, H^{[f_{\rm op}]\text{space-scalar}}_{0;\mathcal{C}\mathcal{M}_\mathcal{C}}|[f]\alpha\beta LSJM_JTM_T\rangle$$

$$= \tfrac{1}{2}n(n-1)\delta_{[f][f']}\delta_{\alpha\alpha'}\delta_{SS'}\delta_{LL'}\sum_{[f^{(n-2)}][f^{(2)}]}\frac{\mathcal{N}_{[f^{(n-2)}]}}{\mathcal{N}_{[f]}}\frac{\langle [f^{(2)}]\|\, h^{[f_{\rm op}]}\|[f^{(2)}]\rangle}{[\dim [f_{\rm op}]]^{\frac{1}{2}}}$$

$$\times \sum_\rho \frac{U([f][f^{(2)*}][f][f^{(2)}];\,[f^{(n-2)}];\,[f_{\rm op}]\rho)}{U([f][f^{(2)*}][f][f^{(2)}];\,[f^{(n-2)}];\,[0])}\langle [f]\beta ST;\,[f_{\rm op}]0\mathcal{C}\,\|\,[f]\beta'ST'\rangle_\rho\langle TM_T\mathcal{C}\mathcal{M}_\mathcal{C}\,|\,T'M'_T\rangle. \quad (69)$$

If the operator is also an isoscalar (charge-independent)—that is, if $\mathcal{S} = 0$ *and* $\mathcal{C} = 0$—then the $SU(4)$ tensor character is restricted to $[f_{\rm op}] = [0]$, $[22]$, or $[422]$. For the special $SU(4)$ representations of Sec. 3 the multiplicity label ρ is needed only for the case $[f_{\rm op}] = [422]$. In this case the quantum number was chosen such that the (S, T)-dependence of the matrix element is given solely by the $SU(4)$ Wigner coefficients with $\rho = 1$; that is,

$$\sum_{[f^{(n-2)}]}\frac{\mathcal{N}_{[f^{(n-2)}]}}{\mathcal{N}_{[f]}}\frac{U([f][2^3][f][2];\,[f^{(n-2)}];\,[422]\rho)}{U([f][2^3][f][2];\,[f^{(n-2)}];\,[0])} = 0 \quad \text{for } \rho \neq 1. \quad (70)$$

In the case of complete space-scalar, charge-independent operators, however, the matrix elements (69) have a very simple form which can be derived by much more elementary techniques. A complete space-scalar, charge-independent two-body operator can be expressed in terms of the operators

$$\sum_{i<j}\tfrac{1}{2}(1 \pm P^{(\rm space)}_{ij}),\quad \sum_{i<j}(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j),\quad \sum_{i<j}(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j), \quad (71)$$

where $P^{(\rm space)}_{ij}$ is the Majorana or space exchange operator. These have the corresponding well-known eigenvalues

$$n_\pm,\quad 2[S(S+1) - \tfrac{3}{4}n],\quad 2[T(T+1) - \tfrac{3}{4}n], \quad (72)$$

where n_+ (n_-) are the number of *spacially* symmetrically (or antisymmetrically) coupled pairs of nucleons in the n-nucleon state, where[21]

$$n_\pm = \tfrac{1}{4}n(n-1) \mp \tfrac{1}{4}[\tfrac{1}{4}n^2 - 4n + C(SU_4)]. \quad (73)$$

The $SU(4)$ irreducible tensor form of these operators is given by

$$T^{[0]} = \sum_{i<j}[(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j) + (\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j) + (\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)];\quad \text{or } \sum_{i<j}1,$$

$$T^{[22]} = \sum_{i<j}[(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j) - (\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)], \quad (74)$$

$$T^{[422]} = \sum_{i<j}[\tfrac{2}{3}(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j) - (\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j) - (\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)].$$

If the two-body operator includes the Coulomb interaction so that it can have isovector ($\mathcal{C} = 1$) and isotensor ($\mathcal{C} = 2$) components, the matrix elements (68) and (69) are much more complicated, and their evaluation in general form involves the full $SU(4)$ machinery. The isovector part has $SU(4)$ tensor character [211], and both $SU(4)$ Wigner and Racah coefficients with $\rho = 1$ and $\rho \neq 1$ make a contribution to the matrix elements of the n-nucleon system. The isotensor part will receive contributions from operators with $SU(4)$ tensor character [22] and [422].

[21] J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1960), p. 239.

5.4. Coulomb Interaction

The Coulomb energy in nuclei seems to show only a relatively mild dependence on the spatial quantum numbers, and it may be a good approximation to replace the full Coulomb interaction energy by the diagonal matrix elements of the complete space-scalar part of the interaction,[9] particularly if the motivation focuses on a study of the dependence of the Coulomb interaction on nucleon number and the spin–isospin, and Wigner supermultiplet quantum numbers.[9]

The diagonal matrix element of the full Coulomb interaction

$$V_C = \sum_{i<j} \frac{e^2}{r_{ij}} [\tfrac{1}{3}(\tfrac{3}{4} + \mathbf{t}_i \cdot \mathbf{t}_j) - \tfrac{1}{2}(t_{z_i} + t_{z_j}) + \tfrac{1}{3}(3t_{z_i}t_{z_j} - \mathbf{t}_i \cdot \mathbf{t}_j)] \quad (75)$$

leads to the Coulomb energy formula

$$E_C = E_C^{(0)} - M_T E_C^{(1)} + [3M_T^2 - T(T+1)]E_C^{(2)}. \quad (76)$$

The Coulomb interaction can be decomposed into irreducible tensor operators of the type $H^{[f_{op}]}_{S;\mathfrak{C}\mathcal{M}_{\mathfrak{C}}} = H^{[f_{op}]}_{0;\mathfrak{C}0}$, defined in Eq. (66). The full decomposition is given in Ref. 9. The complete space-scalar part of the Coulomb interaction can be expressed as

$$V_C^{\text{space-scalar}} = \alpha\left\{\frac{1}{\sqrt{6}}(H'^{[0]}_{0;00} + H'^{[22]}_{0;00}) - \frac{1}{\sqrt{2}} H'^{[211]}_{0;10} - \frac{1}{\sqrt{6}} H'^{[22]}_{0;20}\right\} + \beta\left\{\frac{1}{\sqrt{10}}(3H''^{[0]}_{0;00} + H''^{[422]}_{0;00}) + \sqrt{\tfrac{3}{2}}\, H''^{[211]}_{0;10} + \frac{1}{\sqrt{2}} H''^{[422]}_{0;20}\right\}, \quad (77)$$

where the coefficients α and β must be calculated for each major oscillator shell. [Results for the $1p$ and $2s$, $1d$ shells are given in Ref. 9. Equation (6b) of Ref. 9 should read $\alpha = 127/96$, $\beta = 7/6$.] The two-body operators H' (characterized by a single prime) are built from pair operators $a^\dagger a^\dagger$, (aa), with $SU(4)$ tensor character [11], while the two-body operators H'' (characterized by a double prime) are built from pair operators $a^\dagger a^\dagger$, (aa), with $SU(4)$ tensor character [2], ([2³]). These operators have two-particle reduced matrix elements

$$\langle [11] \| h'^{[f_{op}]} \| [11] \rangle = \left[\frac{\dim [f_{op}]}{\dim [11]}\right]^{\frac{1}{2}},$$
$$\langle [2] \| h''^{[f_{op}]} \| [2] \rangle = \left[\frac{\dim [f_{op}]}{\dim [2]}\right]^{\frac{1}{2}}. \quad (78)$$

In the approximation in which the full Coulomb energy is replaced by its complete space-scalar part, the coefficients $E_C^{(0)}$, $E_C^{(1)}$, and $E_C^{(2)}$ of Eq. (76) can now be evaluated with the aid of Eqs. (69), (77), and (78). The isoscalar coefficient $E_C^{(0)}$ can also be evaluated by more elementary techniques, Eqs. (71)–(74). It has the value

$$E_C^{(0)} = \frac{(\alpha + 3\beta)}{16} \tfrac{1}{2} n(n-1) + \frac{(\alpha + 3\beta)}{24}[T(T+1) - \tfrac{3}{4}n] - \frac{(\alpha - \beta)}{24}[C(SU_4) + 2S(S+1) - T(T+1) - \tfrac{9}{2}n] + \tfrac{3}{2} n a_c. \quad (79)$$

The isovector and isotensor coefficients can be calculated with the aid of the expressions for the $SU(4)$ Wigner and Racah coefficients needed for the evaluation of (69). These are given in Appendix B, which includes tabulations of the diagonal coefficients

$$\langle [f]ST; [f_{op}]0\mathfrak{C} \parallel [f]ST \rangle_\rho$$

with $[f_{op}] = [211]$, $[22]$, and $[422]$, and the needed Racah coefficients, including the sums

$$\Sigma_2 = \tfrac{1}{2} n(n-1) \sum_{[f^{(n-2)}]} \frac{\mathcal{N}_{[f^{(n-2)}]}}{\mathcal{N}_{[f]}} \times \frac{U([f][f^{(2)*}][f][f^{(2)}]; [f^{(n-2)}]; [f_{op}]\rho)}{U([f][f^{(2)*}][f][f^{(2)}]; [f^{(n-2)}]; [0])}. \quad (80)$$

Results for the isovector and isotensor Coulomb energy coefficients $E_C^{(1)}$ and $E_C^{(2)}$ are collected in Table X. Some of these results have been given previously[9] in a somewhat different form. It is convenient to express the Coulomb energy coefficients in terms of the parameters

$$b = \tfrac{1}{24}(\alpha + 3\beta), \quad c = \tfrac{1}{48}(\alpha - \beta), \quad (81)$$

and a parameter a_c which gives the contribution from the interaction of the n nucleons in the partially filled major oscillator shell with those of the core.[9] The coefficients c are of the order of 5 to 10 kev for the $1p$ and $2s$, $1d$ shells, while b is of the order of 50–100 kev.[22] Since the dependence on the spin–isospin and Wigner supermultiplet quantum numbers is given entirely by the c terms, it can be seen that the Coulomb energy shows only a mild dependence on the quantum numbers y, S, T. If the integers y are related to nucleon number n, it can be seen that the nature of

[22] J. Jänecke, in *Isospin in Nuclear Physics*, D. H. Wilkinson, Ed. (North-Holland Publishing Co., to be published).

TABLE X. Isovector and isotensor Coulomb energy coefficients.[a]

$SU(4)$ Rep. $[f]$	$SU(4)$ Rep. $(PP'P'')$	$E_0^{(1)}$	$E_0^{(2)}$
$[yy0]$	$(y00)$	$3a_c + 3b(n-1) + 18c$	$b - c + c\dfrac{[(2y+5)(2y+3) - 4S(S+1)]}{(2T-1)(2T+3)}$
$[y\,y-1\,0]$	$(y-\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})$	$3a_c + 3b(n-1) + 18c$	
$[yy1]$	$(y-\frac{1}{2}\,\frac{1}{2}-\frac{1}{2})$	$-6cz\dfrac{[(2y+3)+(-1)^{y-S-T}(2S+1)(2T+1)]}{4T(T+1)}$	$b - c + c\dfrac{[(y+2)(y+1) - S(S+1)]}{T(T+1)}$
$[y00]$	$(\frac{1}{2}y\,\frac{1}{2}y\,\frac{1}{2}y)$	$3a_c + 3b(n-1) + 18c$	
$[yyy]$	$(\frac{1}{2}y\,\frac{1}{2}y-\frac{1}{2}y)$	$-6cz(y+2)$	$b - 2c$
$[y11]$	$(\frac{1}{2}y\,\frac{1}{2}y\,\frac{1}{2}y-1)$	$3a_c + 3b(n-1) + 18c$ for	for
$[y\,y-1\,y-1]$	$(\frac{1}{2}y\,\frac{1}{2}y-(\frac{1}{2}y-1))$	$+6cz\begin{cases}\dfrac{(y+2)}{T(T+1)} - y & \leftarrow S=T\\ \dfrac{(y+2)}{T} - (y+2) & \leftarrow S=T-1\\ \dfrac{-(y+2)}{T+1} - (y+2) & \leftarrow S=T+1\end{cases}$	$b - 2c + 2c\begin{cases}\dfrac{(y+2)}{T(T+1)} & S=T\\ -\dfrac{[(y+2)-2T]}{(2T-1)T} & S=T-1\\ -\dfrac{[(y+2)+2(T+1)]}{(2T+3)(T+1)} & S=T+1\end{cases}$

[a] $z = (P''/|P''|)$. n = number of nucleons in a major oscillator shell.

the (n, T)-dependent terms for the Wigner supermultiplet scheme are very similar to those predicted for the low v limit of the seniority scheme.[9] The results of Table X thus seem to indicate that the major (n, T)-dependent effects in the systematics of Coulomb displacement energies are quite insensitive to the exact nature of the wavefunctions of the n-nucleon system.

6. CONCLUDING REMARKS

In principle, it is possible to extend the techniques used in this investigation for $SU(4)$ to the unitary groups needed to classify the space parts of the wavefunctions, such as $SU(3)$ and $SU(6)$ for the $1p$ and $2s$, $1d$ shells, for example. In principle, therefore, the full cfp expansions can be summed in general, and the matrix elements of one- and two-body operators can be expressed entirely in terms of Wigner and Racah coefficients for the special unitary groups. In the most general case, however, the algebraic nature of such coefficients is again very complicated,[23] and the expressions for the matrix elements are severely complicated by the multiplicity problem and the sums over the multiplicity labels. It may, however, again be possible to single out certain simple representations of special interest for which the summations over both the spin–isospin and space quantum numbers can be carried out in the cfp expansions for the matrix elements. The resultant interplay between the Wigner supermultiplet and the spacial quantum numbers may lead to interesting studies.

ACKNOWLEDGMENT

It is a pleasure to thank Y. Akiyama for a careful reading of the manuscript.

APPENDIX A. CALCULATION OF NORMALIZATION COEFFICIENTS

To illustrate the technique used in the calculation of the normalization coefficients associated with the step operators $O_{\alpha\beta}$, Eqs. (11) and Table VII, the details of the calculation will be sketched for two of the representations of Sec. 3, viz., $[yy0]$ and $[y\,y-1\,0]$. In order to evaluate the normalization constants for the step operators $O_{\alpha\beta}$ it is necessary to evaluate matrix elements of the type

$$\langle [f]\{ST\}|\, E_{-\alpha-\beta}E_{\alpha\beta}\,|[f]\{ST\}\rangle \equiv (\overline{E_{-\alpha-\beta}E_{\alpha\beta}}). \quad \text{(A1)}$$

The curly bracket is again used to denote states with $M_s = S$, $M_T = T$. There are altogether five independent types of such matrix elements, those with $\alpha\beta = 11$, $1-1$, 10, 01, and 00, respectively. One relation among the five can be obtained from the expression for the quadratic Casimir operator, Eq. (22b), which gives

$$2[(\overline{E_{-1-1}E_{11}}) + (\overline{E_{-11}E_{1-1}}) + (\overline{E_{-10}E_{10}}) + (\overline{E_{0-1}E_{01}})] + (\overline{E_{00}E_{00}}) = C(SU_4) - S^2 - T^2 - 4S - 2T. \quad \text{(A2)}$$

The further evaluation of the matrix elements proceeds differently for the different irreducible representations.

The Representation $[yy0]$

In this representation the possible ST values (Table IV) are such that $y - S - T$ = even integer. Neighbor states thus have the property $|\Delta S| + |\Delta T| = 2$, so that

$$O_{\alpha\beta}\,|[yy0]\{ST\}\rangle = 0 \quad \text{if} \quad |\alpha| + |\beta| = 1. \quad \text{(A3)}$$

[23] J. D. Vergados, Nucl. Phys. A111, 681 (1968).

This implies

$$\langle [yy0]\{ST\}|\, O_{-\alpha-\beta}O_{\alpha\beta}\,|[yy0]\{ST\}\rangle = 0 \quad \text{for } |\alpha| + |\beta| = 1. \tag{A4}$$

With the relations of Tables II and III and the commutation properties of the infinitesimal operators, the four equations (A4) lead to four relations among the matrix elements (A1):

$$(\overline{E_{-10}E_{10}}) = (\overline{E_{-1-1}E_{11}})\frac{1}{(T+1)},$$

$$(\overline{E_{0-1}E_{01}}) = (\overline{E_{-1-1}E_{11}})\frac{1}{(S+1)},$$

$$(\overline{E_{-10}E_{10}}) + (\overline{E_{0-1}E_{01}})\frac{1}{S(T+1)} - (\overline{E_{-11}E_{1-1}})\frac{1}{(T+1)} - (\overline{E_{00}E_{00}})\frac{1}{S} + \frac{T(S+1)}{(T+1)} = 0,$$

$$(\overline{E_{-10}E_{10}})\frac{1}{T(S+1)} + (\overline{E_{0-1}E_{01}}) - (\overline{E_{-11}E_{1-1}})\frac{1}{(S+1)} - (\overline{E_{00}E_{00}})\frac{1}{T} + T = 0. \tag{A5}$$

Together with (A2) these furnish the five equations needed to evaluate the matrix elements (A1) as functions of y, S, and T. In particular,

$$(\overline{O_{-1-1}O_{11}}) = (\overline{E_{-1-1}E_{11}}) = \frac{(S+1)(T+1)(y-S-T)(y+S+T+4)}{(2S+3)(2T+3)}, \tag{A6}$$

$$(\overline{O_{-11}O_{1-1}}) = (\overline{E_{-11}E_{1-1}}) - \frac{(\overline{E_{-1-1}E_{11}})}{(T+1)(2T+1)} = \frac{T(S+1)(y+3+S-T)(y+1-S+T)}{(2S+3)(2T+1)}, \tag{A7}$$

which lead to the normalization coefficients of Table VII.

The Representation $[y\ y-1\ 0]$

The unit step operators $O_{\alpha 0}$, $O_{0\alpha}$ do not give zero when acting on the states of the representation $[y\ y-1\ 0]$, so that the construction of the state vectors is more complicated than in the previous example. However, from the relations

$$\langle [y\ y-1\ 0]\{ST\}|\, O_{-\alpha-\beta}O_{\alpha\beta}\,|[y\ y-1\ 0]\{ST\}\rangle = \langle [y\ y-1\ 0]\{S+\alpha, T+\beta\}| \times O_{\alpha\beta}O_{-\alpha-\beta}\,|[y\ y-1\ O]\{S+\alpha, T+\beta\}\rangle \tag{A8}$$

with the four $\alpha\beta$ values 11, 1 − 1, 10, and 01, four equations are obtained, which, together with (A2), are sufficient to determine the five needed matrix elements. Equations (A8) are essentially recursion equations relating matrix elements of states with $S+T = y-(k-1)$ (states shown in the kth column of Table V) to matrix elements of states with $S+T = y-(k-1)+\alpha+\beta$ [states in the $(k-\alpha-\beta)$th column of Table V]. General expressions for the matrix elements must thus be evaluated through recursion techniques. For this purpose it is convenient to expand the shorthand notation of Eq. (A1) with a subscript k for states with $S+T = y-(k-1)$, identifying the corresponding kth column of Table V. The recursive process is sketched in this section.

Matrix Elements for States with $k = 1$: $S+T = y$

Since E_{11}, E_{10}, E_{01} give zero when operating on states with $k = 1$,

$$(\overline{E_{-1-1}E_{11}})_1 = (\overline{E_{-10}E_{10}})_1 = (\overline{E_{0-1}E_{01}})_1 = 0. \tag{A9a}$$

Also, E_{00} commutes with E_{-11}, which is equivalent to O_{-11} when acting on states with $k = 1$. The matrix element $(\overline{E_{00}E_{00}})_1$ is thus independent of S and T and can be evaluated from (A2) applied to the highest weight state. This gives $(\overline{E_{00}E_{00}})_1 = \frac{1}{4}$. With these four matrix elements (A2) can be used to evaluate

$$(\overline{E_{-11}E_{1-1}})_1 = (S+\tfrac{1}{2})(T-\tfrac{1}{2}) \quad \text{with} \quad S+T = y. \tag{A9b}$$

With the relations of Tables II and III these lead to

$$(\overline{O_{-11}O_{1-1}})_1 = (S+\tfrac{1}{2})(T-\tfrac{1}{2}),$$
$$(\overline{O_{11}O_{-1-1}})_1 = \frac{(S-\tfrac{1}{2})(T-\tfrac{1}{2})(S+T+1)}{ST},$$
$$(\overline{O_{10}O_{-10}})_1 = \frac{(S-\tfrac{1}{2})(S+T+1)}{2S(T+1)}, \tag{A10}$$
$$(\overline{O_{01}O_{0-1}})_1 = \frac{(T-\tfrac{1}{2})(S+T+1)}{2T(S+1)}.$$

Matrix Elements for States with $k = 2$: $S+T = y-1$

The basic recursion relation (A8) gives

$$(\overline{O_{0-1}O_{01}})_2 = \langle \{S, T+1\}|\, O_{01}O_{0-1}\,|\{S, T+1\}\rangle_{k=1} = \frac{(T+\tfrac{1}{2})(S+T+2)}{2(T+1)(S+1)}, \tag{A11a}$$

$$(\overline{O_{-10}O_{10}})_2 = \langle \{S+1, T\}|\, O_{10}O_{-10}\,|\{S+1, T\}\rangle_{k=1} = \frac{(S+\tfrac{1}{2})(S+T+2)}{2(S+1)(T+1)}, \tag{A11b}$$

where the right-hand side follows from (A10). Also, since states with $S+T = y+1$ do not exist,

$$(\overline{O_{-1-1}O_{11}})_2 = 0. \tag{A11c}$$

Finally, setting $\alpha\beta = 1 - 1$ in the recursion relation (A8), and using the relations of Table II together with the commutation properties of the operators and the results (A11), a recursion relation is obtained for the matrix elements $\overline{(E_{-11}E_{1-1})_2}$:

$$\langle\{ST\}|\, E_{-11}E_{1-1}\,|\{ST\}\rangle_{k=2} = \langle\{S+1, T-1\}|\, E_{-11}E_{1-1}\,|\{S+1, T-1\}\rangle_{k=2} + \frac{(y+1)(y+\frac{1}{2})(S-T+1)}{2(S+1)(S+2)T(T+1)} + (S-T+2). \tag{A12}$$

With the initial term

$$\langle\{y-\tfrac{3}{2}, \tfrac{1}{2}\}|\, E_{-11}E_{1-1}\,|\{y-\tfrac{3}{2}, \tfrac{1}{2}\}\rangle_2 = \frac{2(y-1)(y+1)}{3(y-\frac{1}{2})}, \tag{A13}$$

which follows from $O_{1-1}\,|\{y-\frac{3}{2}, \frac{1}{2}\}\rangle = 0$, the result of the recursion process gives

$$\overline{(E_{-11}E_{1-1})_2} = \frac{(S+\frac{1}{2})(T+\frac{1}{2})(S+T+2)}{(S+1)(T+1)} + (S+\tfrac{1}{2})(T-\tfrac{1}{2}). \tag{A14}$$

This result, together with Eqs. (A11) and (A2) leads to the five basic matrix elements $\overline{(E_{-\alpha-\beta}E_{\alpha\beta})_2}$ and the remaining matrix elements $\overline{(O_{-\alpha-\beta}O_{\alpha\beta})_2}$ with $\alpha\beta = -1-1, -10, 0-1, -11$.

Matrix Elements for States of Arbitrary k

The recursion equation (A8) relates the matrix elements $\overline{(O_{-1-1}O_{11})_k}$ to those of type $\overline{(O_{11}O_{-1-1})_{k-2}}$, and the matrix elements $\overline{(O_{-10}O_{10})_k}$ and $\overline{(O_{0-1}O_{01})_k}$ to those of type $\overline{(O_{10}O_{-10})_{k-1}}$ and $\overline{(O_{01}O_{0-1})_{k-1}}$. Since matrix elements for states in the $(k-1)$th and $(k-2)$th column of Table V are known, the matrix elements $\overline{(E_{-\alpha-\beta}E_{\alpha\beta})_k}$ with $\alpha\beta = 11$, 10, and 01 can be evaluated. Matrix elements $\overline{(E_{-11}E_{1-1})_k}$ are evaluated from the recursion equation which is the analog of (A12), while those with $\alpha\beta = 00$ then follow from Eq. (A2). From the five basic matrix elements all others follow.

APPENDIX B. TABLES OF $SU(4)$ WIGNER AND RACAH COEFFICIENTS

The $SU(4)$ Wigner coefficients tabulated are those involving products of the special $SU(4)$ representations enumerated in Sec. 3 with the representations [1], and [2] or [11], needed for one- and two-particle cfp's, as well as products with [211], [22], and [422]. Wigner coefficients involving the coupling with [22] and [422] include only the coefficients for the diagonal matrix elements of the corresponding two-body operators used in the applications. In those special cases where the $SU(4)$ Wigner coefficients coincide with the numerical tabulations of Jahn and coworkers,[2,24] there are differences in the phases of the coefficients. Unfortunately, there is no simple relationship between the phase conventions used in this work and the earlier ones of Ref. 2 (which involve many arbitrary choices of sign).

The tables of $SU(4)$ Wigner coefficients are preceded by Table A.0 listing all of the cases covered in the subsequent tables. Other coefficients can be obtained from these through the symmetry properties (I)–(III), Eqs. (38)–(40), and (38′).

The $SU(4)$ U coefficients tabulated are those needed to evaluate diagonal matrix elements of one- and two-body operators; that is,

$$U([f][f^{(2)*}][f][f^{(2)}];\, [f^{(12)}];\, [f_{\rm op}]\rho)$$

with $[f^{(2)}] = [1]$, and [2], or [11], Tables VII and VIII, respectively. The tables include the sums

$$\Sigma_1 = n \sum_{[f^{(n-1)}]} \frac{\mathcal{N}_{[f^{(n-1)}]}}{\mathcal{N}_{[f]}} \times \frac{U([f][1^3][f][1];\, [f^{(n-1)}];\, [f_{\rm op}]\rho)}{U([f][1^3][f][1];\, [f^{(n-1)}];\, [0])} \tag{B1}$$

and

$$\Sigma_2 = \tfrac{1}{2}n(n-1) \sum_{[f^{(n-2)}]} \frac{\mathcal{N}_{[f^{(n-2)}]}}{\mathcal{N}_{[f]}} \times \frac{U([f][f^{(2)*}][f][f^{(2)}];\, [f^{(n-2)}];\, [f_{\rm op}]\rho)}{U([f][f^{(2)*}][f][f^{(2)}];\, [f^{(n-2)}][0])} \tag{B2}$$

with $[f^{(2)}] = [2]$ or [11]. The summations are over all possible values of $[f^{(n-1)}]$ or $[f^{(n-2)}]$, that is, over all possible rows of Tables VII and VIII. $\mathcal{N}_{[f]}$ denotes the dimension of the irreducible representation of the symmetric group on n objects described by the Young tableau $[f]$.

The sums Σ_1 are expressed in general form in Eq. (59). From the nature of the operators with irreducible tensor character [422] and [22], Eqs. (36) and (74), it can be seen that the sums Σ_2 with $[f_{\rm op}] = [422]$ or [22] can be functions only of the $SU(4)$ quantum numbers and must be independent of nucleon number n. With $[f_{\rm op}] = [211]$, on the other hand, the sums Σ_2 are functions of the full $U(4)$ representation labels. In Tables VIII, the $SU(4)$ irreducible representation labels $[f_1 - f_4, f_2 - f_4, f_3 - f_4]$ are expressed in terms of the integers y. The label f_4 is replaced by the integer x; the full $U(4)$ tableau is assumed to include x columns of 4.

[24] J. P. Elliott, J. Hope, and H. A. Jahn, Phil. Trans. Roy. Soc. London **A246**, 241 (1953).

TABLE A.0. Organization of tables of $SU(4)$ Wigner coefficients. $[f^{(1)}] \times [f^{(2)}] \to [f]$.

$[f^{(1)}]$	$[f^{(2)}]$	$[f]$	Table number
$[yy0]$	[1]	$[y+1\ y0]$, $[yy1]$	A1.1
$[y\ y-1\ 0]$	[1]	$[yy0]$	A1.2
$[yy1]$	[1]	$[y-1\ y-1\ 0]$	A1.3
$[y00]$	[1]	$[y+1\ 00]$, $[y10]$	A1.4
$[y10]$	[1]	$[y+1\ 10]$, $[y11]$	A1.5
$[y11]$	[1]	$[y-1\ 00]$, $[y+1\ 11]$	A1.6
$[yy0]$	[11]	$[y+1\ y+1\ 0]$, $[y-1\ y-1\ 0]$	A2.1
$[y00]$	[11]	$[y+1\ 10]$, $[y11]$	A2.2
$[y\ y-1\ 0]$	[11]	$[y+1\ y0]$, $[yy1]$, $[y-1\ y-2\ 0]$	A2.3
$[y11]$	[11]	$[y-1\ 10]$, $[y00]$	A2.4
$[y\ y-1\ 0]$	[2]	$[y+1\ y0]$, $[yy1]$	A3.1
$[yy1]$	[2]	$[y\ y-1\ 0]$, $[y-1\ y-1\ 1]$	A3.2
$[y00]$	[2]	$[y+1\ 10]$, $[y+2\ 00]$	A3.3
$[y-1\ 10]$	[2]	$[y+1\ 10]$, $[y11]$	A3.4
$[y11]$	[2]	$[y+2\ 11]$, $[y-1\ 10]$, $[y00]$	A3.5
$[yy0]$	[211]	$[yy0]$	A4.1
$[y00]$	[211]	$[y00]$	A4.2
$[y\ y-1\ 0]$	[211]	$[y\ y-1\ 0]$ $\rho=1,2$,	A4.3
$[y\ y-1\ 0]$	[211]	$[y+1\ y+1\ 1]$	A4.4
$[y10]$	[211]	$[y10]$, $\rho=1,2$,	A4.5
$[y11]$	[211]	$[y11]$, $\rho=1,2$	A4.6
$[yy0]$	[22], [422]	$[yy0]$	A5.1, 5.2
$[y00]$	[422]	$[y00]$	A5.3
$[y\ y-1\ 0]$	[22], [422]	$[y\ y-1\ 0]$ $\rho=1,2$	A6.1, 6.2
$[y11]$	[22], [422]	$[y11]$ $\rho=1,2$	A6.3, 6.4

TABLE A1.1.

S_1T_1	$\left\langle \begin{matrix}[yy0]\ [100] \\ S_1T_1;\ \frac{1}{2}\frac{1}{2}\end{matrix} \middle\| \begin{matrix}[y+1\ y0] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[yy0]\ [100] \\ S_1T_1;\ \frac{1}{2}\frac{1}{2}\end{matrix} \middle\| \begin{matrix}[yy1] \\ ST\end{matrix} \right\rangle$
$S+\frac{1}{2}\ T+\frac{1}{2}$	$\left[\frac{(y-S-T+1)}{2(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+S+T+3)}{2(y+2)}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ T-\frac{1}{2}$	$\left[\frac{(y+S+T+3)}{2(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{(y-S-T+1)}{2(y+2)}\right]^{\frac{1}{2}}$
$S+\frac{1}{2}\ T-\frac{1}{2}$	$\left[\frac{(y-S+T+2)}{2(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+S-T+2)}{2(y+2)}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ T+\frac{1}{2}$	$\left[\frac{(y+S-T+2)}{2(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{(y-S+T+2)}{2(y+2)}\right]^{\frac{1}{2}}$

TABLE A1.2.

S_1T_1	$\left\langle \begin{matrix}[y\ y-1\ 0]\ [100] \\ S_1T_1;\ \frac{1}{2}\frac{1}{2}\end{matrix} \middle\| \begin{matrix}[yy0] \\ ST\end{matrix} \right\rangle$
$S+\frac{1}{2}\ T+\frac{1}{2}$	$-\left[\frac{(y-S-T)(S+1)(T+1)}{y(2S+1)(2T+1)}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ T-\frac{1}{2}$	$-\left[\frac{(y+S+T+2)ST}{y(2S+1)(2T+1)}\right]^{\frac{1}{2}}$
$S+\frac{1}{2}\ T-\frac{1}{2}$	$\left[\frac{(y-S+T+1)(S+1)T}{y(2S+1)(2T+1)}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ T+\frac{1}{2}$	$\left[\frac{(y+S-T+1)S(T+1)}{y(2S+1)(2T+1)}\right]^{\frac{1}{2}}$

TABLE A1.3.

S_1T_1	$\left\langle \begin{matrix}[yy1]\ [100] \\ S_1T_1;\ \frac{1}{2}\frac{1}{2}\end{matrix} \middle\| \begin{matrix}[y-1\ y-1\ 0] \\ ST\end{matrix} \right\rangle$
$S+\frac{1}{2}\ T+\frac{1}{2}$	$\left[\frac{(y+S+T+3)(S+1)(T+1)}{(y+3)(2S+1)(2T+1)}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ T-\frac{1}{2}$	$-\left[\frac{(y-S-T+1)ST}{(y+3)(2S+1)(2T+1)}\right]^{\frac{1}{2}}$
$S+\frac{1}{2}\ T-\frac{1}{2}$	$-\left[\frac{(y+S-T+2)(S+1)T}{(y+3)(2S+1)(2T+1)}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ T+\frac{1}{2}$	$\left[\frac{(y-S+T+2)S(T+1)}{(y+3)(2S+1)(2T+1)}\right]^{\frac{1}{2}}$

TABLE A1.4.

S_1T_1	$\left\langle \begin{matrix}[y00]\ [100] \\ S_1T_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[y+1\ 00] \\ ST=S\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[y00]\ [100] \\ S_1T_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[y10] \\ ST=S\end{matrix} \right\rangle$
$S+\frac{1}{2}\ S+\frac{1}{2}$	$\left[\frac{(S+1)(y+1-2S)}{(y+1)(2S+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{S(y+3+2S)}{(y+1)(2S+1)}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ S-\frac{1}{2}$	$\left[\frac{S(y+3+2S)}{(y+1)(2S+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(S+1)(y+1-2S)}{(y+1)(2S+1)}\right]^{\frac{1}{2}}$

$$\left\langle \begin{matrix}[y00]\ [100] \\ S-\frac{1}{2}\ S-\frac{1}{2};\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[y10] \\ S(S-1)\end{matrix} \right\rangle = \left\langle \begin{matrix}[y00]\ [100] \\ S+\frac{1}{2}\ S+\frac{1}{2};\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[y10] \\ S(S+1)\end{matrix} \right\rangle = +1.$$

TABLE A1.5.

S_1T_1	ST	$\left\langle \begin{matrix}[y10]\ [100] \\ S_1T_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[y+1\ 10] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[y10]\ [100] \\ S_1T_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[y11] \\ ST\end{matrix} \right\rangle$
$S+\frac{1}{2}\ S-\frac{1}{2}$	SS	$\frac{1}{(2S+1)}\left[\frac{y+1}{y}\right]^{\frac{1}{2}}$	$\frac{1}{\sqrt{2}}$
$S-\frac{1}{2}\ S+\frac{1}{2}$	SS	$\frac{1}{(2S+1)}\left[\frac{y+1}{y}\right]^{\frac{1}{2}}$	$-\frac{1}{\sqrt{2}}$
$S-\frac{1}{2}\ S-\frac{1}{2}$	SS	$\frac{[(2S-1)(S+1)(y+2+2S)]^{\frac{1}{2}}}{(2S+1)[y]^{\frac{1}{2}}}$	0
$S+\frac{1}{2}\ S+\frac{1}{2}$	SS	$\frac{[(2S+3)S(y-2S)]^{\frac{1}{2}}}{(2S+1)[y]^{\frac{1}{2}}}$	0
$S-\frac{1}{2}\ S-\frac{3}{2}$	$S\ (S-1)$	$\left[\frac{(S-1)(y+2+2S)(y+1)}{(2S-1)y(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(S-1)(y+2-2S)}{2(2S-1)(y+2)}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ S-\frac{1}{2}$	$S\ (S-1)$	$-\left[\frac{(y+2+2S)(y+2-2S)}{(2S-1)(2S+1)y(y+2)}\right]^{\frac{1}{2}}$	$\frac{-S[2(y+1)]^{\frac{1}{2}}}{[(2S-1)(2S+1)(y+2)]^{\frac{1}{2}}}$
$S+\frac{1}{2}\ S-\frac{1}{2}$	$S\ (S-1)$	$\left[\frac{(S+1)(y+2-2S)(y+1)}{(2S+1)y(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{(S+1)(y+2+2S)}{2(2S+1)(y+2)}\right]^{\frac{1}{2}}$

$$\left\langle \begin{matrix}[y10]\ [100] \\ T_1S_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[y+1\ 10] \\ (S-1)S\end{matrix} \right\rangle = \left\langle \begin{matrix}[y10]\ [100] \\ S_1T_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[y+1\ 10] \\ S(S-1)\end{matrix} \right\rangle, \left\langle \begin{matrix}[y10]\ [100] \\ T_1S_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[y11] \\ (S-1)S\end{matrix} \right\rangle = -\left\langle \begin{matrix}[y10]\ [100] \\ S_1T_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[y11] \\ S(S-1)\end{matrix} \right\rangle.$$

TABLE A1.6.

S_1T_1	ST	$\left\langle \begin{matrix}[y11]\ [100] \\ S_1T_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[(y-1)\ 00] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[y11]\ [100] \\ S_1T_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[(y+1)\ 11] \\ ST\end{matrix} \right\rangle$
$S+\frac{1}{2}\ S+\frac{1}{2}$	SS	$\frac{1}{(2S+1)}\left[\frac{(S+1)(2S+3)(y+3+2S)}{3(y+3)}\right]^{\frac{1}{2}}$	$\frac{1}{(2S+1)}\left[\frac{S(2S+3)(y+1-2S)(y+2)}{y(y+3)}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ S-\frac{1}{2}$	SS	$\frac{-1}{(2S+1)}\left[\frac{S(2S-1)(y+1-2S)}{3(y+3)}\right]^{\frac{1}{2}}$	$\frac{1}{(2S+1)}\left[\frac{(S+1)(2S-1)(y+3+2S)(y+2)}{y(y+3)}\right]^{\frac{1}{2}}$
$S+\frac{1}{2}\ S-\frac{1}{2}$	SS	$\frac{2}{(2S+1)}\left[\frac{S(S+1)(y+2)}{3(y+3)}\right]^{\frac{1}{2}}$	$\frac{-1}{(2S+1)}\left[\frac{(y+1-2S)(y+3+2S)}{y(y+3)}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ S+\frac{1}{2}$	SS	$\frac{2}{(2S+1)}\left[\frac{S(S+1)(y+2)}{3(y+3)}\right]^{\frac{1}{2}}$	$\frac{-1}{(2S+1)}\left[\frac{(y+1-2S)(y+3+2S)}{y(y+3)}\right]^{\frac{1}{2}}$
$S+\frac{1}{2}\ S-\frac{1}{2}$	$S\ (S-1)$		$\left[\frac{(S+1)(y+1-2S)}{(2S+1)y}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ S-\frac{1}{2}$	$S\ (S-1)$		$\left[\frac{(y+2)}{y(2S-1)(2S+1)}\right]^{\frac{1}{2}}$
$S-\frac{1}{2}\ S-\frac{3}{2}$	$S\ (S-1)$		$\left[\frac{(S-1)(y+1+2S)}{(2S-1)y}\right]^{\frac{1}{2}}$

$$\left\langle \begin{matrix}[y11]\ [100] \\ T_1S_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[(y+1)11] \\ (S-1)S\end{matrix} \right\rangle = \left\langle \begin{matrix}[y11]\ [100] \\ S_1T_1;\ \frac{11}{22}\end{matrix} \middle\| \begin{matrix}[(y+1)11] \\ S(S-1)\end{matrix} \right\rangle.$$

TABLE A2.1.

$S_1T_1;\ S_2T_2$	$\left\langle \begin{matrix}[yy0]\ [110] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y+1\ y+1\ 0] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[yy0]\ [110] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y-1\ y-1\ 0] \\ ST\end{matrix} \right\rangle$
$S+1\ T;\ 10$	$-\left[\frac{(S+1)(y-S+T+2)(y-S-T+1)}{2(y+1)(y+2)(2S+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(S+1)(y+S-T+2)(y+S+T+3)}{2(y+2)(y+3)(2S+1)}\right]^{\frac{1}{2}}$
$S\ T+1;\ 01$	$-\left[\frac{(T+1)(y+S-T+2)(y-S-T+1)}{2(y+1)(y+2)(2T+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(T+1)(y-S+T+2)(y+S+T+3)}{2(y+2)(y+3)(2T+1)}\right]^{\frac{1}{2}}$
$S\ T-1;\ 01$	$\left[\frac{T(y+S+T+3)(y-S+T+2)}{2(y+1)(y+2)(2T+1)}\right]^{\frac{1}{2}}$	$\left[\frac{T(y-S-T+1)(y+S-T+2)}{2(y+2)(y+3)(2T+1)}\right]^{\frac{1}{2}}$
$S-1\ T;\ 10$	$\left[\frac{S(y+S+T+3)(y+S-T+2)}{2(y+1)(y+2)(2S+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{S(y-S-T+1)(y-S+T+2)}{2(y+2)(y+3)(2S+1)}\right]^{\frac{1}{2}}$

TABLE A2.2.

$S_1T_1;$	$S_2T_2\ ST$	$\left\langle \begin{matrix}[y00]\ [110] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y+1\ 10] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[y00]\ [110] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y11] \\ ST\end{matrix} \right\rangle$
$SS;$	$10\ SS$	$-1/\sqrt{2}$	$1/\sqrt{2}$
$SS;$	$01\ SS$	$-1/\sqrt{2}$	$-1/\sqrt{2}$
$S-1\ S-1;$	$10\ S(S-1)$	$\left[\frac{y+2+2S}{2(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{y+2-2S}{2(y+2)}\right]^{\frac{1}{2}}$
$SS;$	$01\ S(S-1)$	$-\left[\frac{y+2-2S}{2(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{y+2+2S}{2(y+2)}\right]^{\frac{1}{2}}$
$S+1\ S+1;$	$10\ S(S+1)$	$-\left[\frac{y-2S}{2(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{y+4+2S}{2(y+2)}\right]^{\frac{1}{2}}$
$SS;$	$01\ S(S+1)$	$\left[\frac{y+4+2S}{2(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{y-2S}{2(y+2)}\right]^{\frac{1}{2}}$

TABLE A2.3. $\left\langle \begin{matrix} [y\ y-1\ 0]\ [110] \\ S_1T_1;\ S_2T_2 \end{matrix} \middle\| \begin{matrix} [f'] \\ ST \end{matrix} \right\rangle$.

$S_1T_1;\ S_2T_2$	$[f'] = [y+1\ y0]$	$[f'] = [yy1]$	$[f'] = [y-1\ y-2\ 0]$
	(a) $y - S - T =$ even integer		
$S+1\ T;\ 10$	$-\left[\frac{(2S+3)(y-S-T)(y-S+T+2)}{8y(y+2)(S+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S+3)(y-S-T)(y+S-T+2)}{16(y+1)(y+2)(S+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S+3)(y+S+T+2)(y+S-T+2)}{8(y+1)(y+3)(S+1)}\right]^{\frac{1}{2}}$
$ST;\ 10$	$-\left[\frac{(y-S+T+2)(y+S-T+2)}{8y(y+2)S(S+1)}\right]^{\frac{1}{2}}$	$\frac{\{(y+1)(2S+1)+S+T+1\}}{4[(y+1)(y+2)S(S+1)]^{\frac{1}{2}}}$	$\left[\frac{(y+S+T+2)(y-S-T)}{8(y+1)(y+3)S(S+1)}\right]^{\frac{1}{2}}$
$S-1\ T;\ 10$	$\left[\frac{(2S-1)(y+S+T+2)(y+S-T+2)}{8y(y+2)S}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S-1)(y+S+T+2)(y-S+T+2)}{16(y+1)(y+2)S}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S-1)(y-S-T)(y-S+T+2)}{8(y+1)(y+3)S}\right]^{\frac{1}{2}}$
$S\ T+1;01$	$-\left[\frac{(2T+3)(y-S-T)(y+S-T+2)}{8y(y+2)(T+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(2T+3)(y-S-T)(y-S+T+2)}{16(y+1)(y+2)(T+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2T+3)(y+S+T+2)(y-S+T+2)}{8(y+1)(y+3)(T+1)}\right]^{\frac{1}{2}}$
$ST;01$	$-\left[\frac{(y+S-T+2)(y-S+T+2)}{8y(y+2)T(T+1)}\right]^{\frac{1}{2}}$	$\frac{-\{(y+1)(2T+1)+S+T+1\}}{4[(y+1)(y+2)T(T+1)]^{\frac{1}{2}}}$	$-\left[\frac{(y-S-T)(y+S+T+2)}{8(y+1)(y+3)T(T+1)}\right]^{\frac{1}{2}}$
$S\ T-1;01$	$\left[\frac{(2T-1)(y+S+T+2)(y-S+T+2)}{8y(y+2)T}\right]^{\frac{1}{2}}$	$\left[\frac{(2T-1)(y+S+T+2)(y+S-T+2)}{16(y+1)(y+2)T}\right]^{\frac{1}{2}}$	$\left[\frac{(2T-1)(y-S-T)(y+S-T+2)}{8(y+1)(y+3)T}\right]^{\frac{1}{2}}$
	(b) $y - S - T =$ odd integer		
$S+1\ T;\ 10$	$-\left[\frac{(2S+3)(y-S-T+1)(y-S+T+1)}{8y(y+2)(S+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S+3)(y-S+T+1)(y+S+T+3)}{16(y+1)(y+2)(S+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S+3)(y+S+T+3)(y+S-T+1)}{8(y+1)(y+3)(S+1)}\right]$
$ST;\ 10$	$-\left[\frac{(y+S+T+3)(y-S-T+1)}{8y(y+2)S(S+1)}\right]^{\frac{1}{2}}$	$\frac{\{(y+1)(2S+1)+S-T\}}{4[(y+1)(y+2)S(S+1)]^{\frac{1}{2}}}$	$\left[\frac{(y-S+T+1)(y+S-T+1)}{8(y+1)(y+3)S(S+1)}\right]^{\frac{1}{2}}$
$S-1\ T;\ 10$	$\left[\frac{(2S-1)(y+S+T+3)(y+S-T+1)}{8y(y+2)S}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S-1)(y+S-T+1)(y-S-T+1)}{16(y+1)(y+2)S}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S-1)(y-S-T+1)(y-S+T+1)}{8(y+1)(y+3)S}\right]^{\frac{1}{2}}$
$S\ T+1;01$	$-\left[\frac{(2T+3)(y-S-T+1)(y+S-T+1)}{8y(y+2)(T+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2T+3)(y+S-T+1)(y+S+T+3)}{16(y+1)(y+2)(T+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2T+3)(y-S+T+1)(y+S+T+3)}{8(y+1)(y+3)(T+1)}\right]^{\frac{1}{2}}$
$ST;01$	$-\left[\frac{(y+S+T+3)(y-S-T+1)}{8y(y+2)T(T+1)}\right]^{\frac{1}{2}}$	$\frac{\{(y+1)(2T+1)-S+T\}}{4[(y+1)(y+2)T(T+1)]^{\frac{1}{2}}}$	$-\left[\frac{(y+S-T+1)(y-S+T+1)}{8(y+1)(y+3)T(T+1)}\right]^{\frac{1}{2}}$
$S\ T-1;01$	$\left[\frac{(2T-1)(y+S+T+3)(y-S+T+1)}{8y(y+2)T}\right]^{\frac{1}{2}}$	$-\left[\frac{(2T-1)(y-S+T+1)(y-S-T+1)}{16(y+1)(y+2)T}\right]^{\frac{1}{2}}$	$\left[\frac{(2T-1)(y-S-T+1)(y+S-T+1)}{8(y+1)(y+3)T}\right]^{\frac{1}{2}}$

TABLE A2.4.

$S_1T_1;$	S_2T_2	ST	$\left\langle \begin{matrix}[y11]\ [110] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y-1\ 10] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[y11]\ [110] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y00] \\ ST\end{matrix} \right\rangle$
$S+1\ S;$	10	SS	$\left[\frac{(2S+3)S(y+2+2S)(y+2)}{4(S+1)(2S+1)y(y+3)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S+3)(y-2S)}{6y(2S+1)}\right]^{\frac{1}{2}}$
$S\ S+1;$	01	SS		
$S\ S;$	10	SS	$\left[\frac{(y-2S)(y+2+2S)}{4S(S+1)y(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{y+2}{6y}\right]^{\frac{1}{2}}$
$S\ S;$	01	SS		
$S-1\ S;$	10	SS	$\left[\frac{(2S-1)(S+1)(y-2S)(y+2)}{4S(2S+1)y(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S-1)(y+2+2S)}{6y(2S+1)}\right]^{\frac{1}{2}}$
$S\ S-1;$	01	SS		
$S\ S-1;$	10	$S(S-1)$	$-\left[\frac{(y+2)(S+1)}{4S(y+3)}\right]^{\frac{1}{2}}$	
$S-1\ S;$	01	$(S-1)S$		
$S-1\ S-1;$	10	$S(S-1)$	$\left[\frac{(S-1)(y+2-2S)}{4S(y+3)}\right]^{\frac{1}{2}}$	
$S-1\ S-1;$	01	$(S-1)S$		
$S\ S;$	01	$S(S-1)$	$\left[\frac{(S+1)(y+2+2S)}{4S(y+3)}\right]^{\frac{1}{2}}$	
$S\ S;$	10	$(S-1)S$		
$S\ S-1;$	01	$S(S-1)$	$\left[\frac{(y+2)(S-1)}{4S(y+3)}\right]^{\frac{1}{2}}$	
$S-1\ S;$	10	$(S-1)S$		

TABLE A3.1.

$S_1T_1;\ S_2T_2$	$\left\langle \begin{matrix}[y\,y-1\,0]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y+1\,y\,0] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[y\,y-1\,0]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[yy1] \\ ST\end{matrix} \right\rangle$
	(a) $y-S-T=$ even integer	
$S+1\ T+1;\ 11$	0	0
$S+1\ T;\ 11$	$-\left[\frac{(2S+3)(T+1)(y-S-T)(y-S+T+2)}{24y(y+2)(S+1)T}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S+3)(T+1)(y-S-T)(y+S-T+2)}{16(y-1)(y+2)(S+1)T}\right]^{\frac{1}{2}}$
$S+1\ T-1;\ 11$	$\left[\frac{(2S+3)(2T-1)(y-S+T)(y-S+T+2)}{24y(y+2)(S+1)T}\right]^{\frac{1}{2}}$	$\left[\frac{(2S+3)(2T-1)(y-S+T)(y+S-T+2)}{16(y-1)(y+2)(S+1)T}\right]^{\frac{1}{2}}$
$S-1\ T+1;\ 11$	$\left[\frac{(2S-1)(2T+3)(y+S-T)(y+S-T+2)}{24y(y+2)S(T+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S-1)(2T+3)(y+S-T)(y-S+T+2)}{16(y-1)(y+2)S(T+1)}\right]^{\frac{1}{2}}$
$S-1\ T;\ 11$	$-\left[\frac{(2S-1)T(y+S+T+2)(y+S-T+2)}{24y(y+2)S(T+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S-1)T(y+S+T+2)(y-S+T+2)}{16(y-1)(y+2)S(T+1)}\right]^{\frac{1}{2}}$
$S-1\ T-1;\ 11$	0	0
$S\ T+1;\ 11$	$-\left[\frac{(S+1)(2T+3)(y-S-T)(y+S-T+2)}{24y(y+2)S(T+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(S+1)(2T+3)(y-S-T)(y-S+T+2)}{16(y-1)(y+2)S(T+1)}\right]^{\frac{1}{2}}$
$S\ T;\ 11$	$\{2ST+S+T\}$ $\times\left[\frac{(y+S-T+2)(y-S+T+2)}{24y(y+2)S(S+1)T(T+1)}\right]^{\frac{1}{2}}$	$\frac{(S-T)\{2ST+S+T+y+2\}}{[16(y-1)(y+2)S(S+1)T(T+1)]^{\frac{1}{2}}}$
$S\ T-1;\ 11$	$-\left[\frac{S(2T-1)(y+S+T+2)(y-S+T+2)}{24y(y+2)(S+1)T}\right]^{\frac{1}{2}}$	$-\left[\frac{S(2T-1)(y+S+T+2)(y+S-T+2)}{16(y-1)(y+2)(S+1)T}\right]^{\frac{1}{2}}$
$S\ T;\ 00$	$\left[\frac{(y+S-T+2)(y-S+T+2)}{6y(y+2)}\right]^{\frac{1}{2}}$	$\frac{(S-T)}{[4(y-1)(y+2)]^{\frac{1}{2}}}$
	(b) $y-S-T=$ odd integer	
$S+1\ T+1;\ 11$	$-\left[\frac{(2S+3)(2T+3)(y-S-T-1)\times(y-S-T+1)}{24y(y+2)(S+1)(T+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S+3)(2T+3)(y-S-T-1)\times(y+S+T+3)}{16(y-1)(y+2)(S+1)(T+1)}\right]^{\frac{1}{2}}$
$S+1\ T;\ 11$	$\left[\frac{(2S+3)T(y-S+T+1)(y-S-T+1)}{24y(y+2)(S+1)(T+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S+3)T(y-S+T+1)(y+S+T+3)}{16(y-1)(y+2)(S+1)(T+1)}\right]^{\frac{1}{2}}$
$S+1\ T-1;\ 11$	0	0
$S-1\ T+1;\ 11$	0	0
$S-1\ T;\ 11$	$\left[\frac{(2S-1)(T+1)(y+S-T+1)\times(y+S+T+3)}{24y(y+2)ST}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S-1)(T+1)(y+S-T+1)\times(y-S-T+1)}{16(y-1)(y+2)ST}\right]^{\frac{1}{2}}$
$S-1\ T-1;\ 11$	$-\left[\frac{(2S-1)(2T-1)(y+S+T+1)\times(y+S+T+3)}{24y(y+2)ST}\right]^{\frac{1}{2}}$	$\left[\frac{(2S-1)(2T-1)(y+S+T+1)\times(y-S-T+1)}{16(y-1)(y+2)ST}\right]^{\frac{1}{2}}$
$S\ T+1;\ 11$	$\left[\frac{S(2T+3)(y+S-T+1)(y-S-T+1)}{24y(y+2)(S+1)(T+1)}\right]^{\frac{1}{2}}$	$\left[\frac{S(2T+3)(y+S-T+1)(y+S+T+3)}{16(y-1)(y+2)(S+1)(T+1)}\right]^{\frac{1}{2}}$
$S\ T;\ 11$	$-\{2ST+S+T+1\}$ $\times\left[\frac{(y+S+T+3)(y-S-T+1)}{24y(y+2)S(S+1)T(T+1)}\right]^{\frac{1}{2}}$	$\frac{(S+T+1)\{y+1-S-T-2ST\}}{[16(y-1)(y+2)S(S+1)T(T+1)]^{\frac{1}{2}}}$
$S\ T-1;\ 11$	$\left[\frac{(S+1)(2T-1)(y-S+T+1)\times(y+S+T+3)}{24y(y+2)ST}\right]^{\frac{1}{2}}$	$-\left[\frac{(S+1)(2T-1)(y-S-T+1)\times(y-S+T+1)}{16(y-1)(y+2)ST}\right]^{\frac{1}{2}}$
$S\ T;\ 00$	$\left[\frac{(y+S+T+3)(y-S-T+1)}{6y(y+2)}\right]^{\frac{1}{2}}$	$\frac{(S+T+1)}{[4(y-1)(y+2)]^{\frac{1}{2}}}$

TABLE A3.2.

$S_1T_1;\quad S_2T_2$	$\left\langle \begin{matrix}[yy1]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y\ y-1\ 0] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[yy1]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y-1\ y-1\ 1] \\ ST\end{matrix} \right\rangle$
	(a) $y - S - T$ = even integer	
$S+1\ T+1;\ 11$	$\left[\frac{(2S+3)(2T+3)(y-S-T)(y+S+T+4)}{16(y+1)(y+4)(S+1)(T+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S+3)(2T+3)(y+S+T+2)\times(y+S+T+4)}{24(y+1)(y+3)(S+1)(T+1)}\right]^{\frac{1}{2}}$
$S+1\ T;\quad 11$	$-\left[\frac{(2S+3)T(y-S-T)(y+S-T+2)}{16(y+1)(y+4)(S+1)(T+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S+3)T(y+S+T+2)(y+S-T+2)}{24(y+1)(y+3)(S+1)(T+1)}\right]^{\frac{1}{2}}$
$S+1\ T-1;\ 11$	0	0
$S-1\ T+1;\ 11$	0	0
$S-1\ T;\quad 11$	$\left[\frac{(2S-1)(T+1)(y-S+T+2)\times(y+S+T+2)}{16(y+1)(y+4)ST}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S-1)(T+1)(y-S-T)(y-S+T+2)}{24(y+1)(y+3)ST}\right]^{\frac{1}{2}}$
$S-1\ T-1;\ 11$	$-\left[\frac{(2S-1)(2T-1)(y-S-T+2)\times(y+S+T+2)}{16(y+1)(y+4)ST}\right]^{\frac{1}{2}}$	$\left[\frac{(2S-1)(2T-1)(y-S-T)(y-S-T+2)}{24(y+1)(y+3)ST}\right]^{\frac{1}{2}}$
$S\ T+1;\ 11$	$\left[\frac{S(2T+3)(y-S-T)(y-S+T+2)}{16(y+1)(y+4)(S+1)(T+1)}\right]^{\frac{1}{2}}$	$\left[\frac{S(2T+3)(y-S+T+2)(y+S+T+2)}{24(y+1)(y+3)(S+1)(T+1)}\right]^{\frac{1}{2}}$
$S\ T;\quad 11$	$\frac{(S+T+1)\{y+2+S+T+2ST\}}{[16(y+1)(y+4)S(S+1)T(T+1)]^{\frac{1}{2}}}$	$-\{2ST+S+T+1\}\times\left[\frac{(y-S-T)(y+S+T+2)}{24(y+1)(y+3)S(S+1)T(T+1)}\right]^{\frac{1}{2}}$
$S\ T-1;\ 11$	$-\left[\frac{(S+1)(2T-1)(y+S+T+2)\times(y+S-T+2)}{16(y+1)(y+4)ST}\right]^{\frac{1}{2}}$	$\left[\frac{(S+1)(2T-1)(y-S-T)(y+S-T+2)}{24(y+1)(y+3)ST}\right]^{\frac{1}{2}}$
$S\ T;\quad 00$	$\frac{-(S+T+1)}{[4(y+1)(y+4)]^{\frac{1}{2}}}$	$\left[\frac{(y-S-T)(y+S+T+2)}{6(y+1)(y+3)}\right]^{\frac{1}{2}}$
	(b) $y - S - T$ = odd integer	
$S+1\ T+1;\ 11$	0	0
$S+1\ T;\quad 11$	$\left[\frac{(2S+3)(T+1)(y-S+T+1)\times(y+S+T+3)}{16(y+1)(y+4)(S+1)T}\right]^{\frac{1}{2}}$	$\left[\frac{(2S+3)(T+1)(y+S+T+3)\times(y+S-T+1)}{24(y+1)(y+3)(S+1)T}\right]^{\frac{1}{2}}$
$S+1\ T-1;\ 11$	$-\left[\frac{(2S+3)(2T-1)(y-S+T+1)\times(y+S-T+3)}{16(y+1)(y+4)(S+1)T}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S+3)(2T-1)(y+S-T+3)\times(y+S-T+1)}{24(y+1)(y+3)(S+1)T}\right]^{\frac{1}{2}}$
$S-1\ T+1;\ 11$	$\left[\frac{(2S-1)(2T+3)(y+S-T+1)\times(y-S+T+3)}{16(y+1)(y+4)S(T+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S-1)(2T+3)(y-S+T+3)\times(y-S+T+1)}{24(y+1)(y+3)S(T+1)}\right]^{\frac{1}{2}}$
$S-1\ T;\quad 11$	$-\left[\frac{(2S-1)T(y-S-T+1)(y+S-T+1)}{16(y+1)(y+4)S(T+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S-1)T(y-S-T+1)(y-S+T+1)}{24(y+1)(y+3)S(T+1)}\right]^{\frac{1}{2}}$
$S-1\ T-1;\ 11$	0	0
$S\ T+1;\ 11$	$\left[\frac{(S+1)(2T+3)(y+S+T+3)\times(y+S-T+1)}{16(y+1)(y+4)S(T+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(S+1)(2T+3)(y+S+T+3)\times(y-S+T+1)}{24(y+1)(y+3)S(T+1)}\right]^{\frac{1}{2}}$
$S\ T;\quad 11$	$\frac{(S-T)\{y+1-S-T-2ST\}}{[16(y+1)(y+4)S(S+1)T(T+1)]^{\frac{1}{2}}}$	$\{2ST+S+T\}\times\left[\frac{(y+S-T+1)(y-S+T+1)}{24(y+1)(y+3)S(S+1)T(T+1)}\right]^{\frac{1}{2}}$
$S\ T-1;\ 11$	$-\left[\frac{S(2T-1)(y-S-T+1)(y-S+T+1)}{16(y+1)(y+4)(S+1)T}\right]^{\frac{1}{2}}$	$-\left[\frac{S(2T-1)(y-S-T+1)(y+S-T+1)}{24(y+1)(y+3)(S+1)T}\right]^{\frac{1}{2}}$
$S\ T;\quad 00$	$\frac{-(S-T)}{[4(y+1)(y+4)]^{\frac{1}{2}}}$	$\left[\frac{(y+S-T+1)(y-S+T+1)}{6(y+1)(y+3)}\right]^{\frac{1}{2}}$

TABLE A3.3.

$S_1T_1;\ S_2T_2$	ST	$\left\langle \begin{matrix}[y00]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y+1\ 10] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[y00]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y+2\ 00] \\ ST\end{matrix} \right\rangle$
$S+1\ S+1;\ 11$	SS	$-\left[\frac{S(2S+3)(y-2S)(y+4+2S)}{2y(y+2)(S+1)(2S+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S+3)(y-2S)(y+2-2S)}{4(y+1)(y+2)(2S+1)}\right]^{\frac{1}{2}}$
$S-1\ S-1;\ 11$	SS	$\left[\frac{(S+1)(2S-1)(y+2+2S)(y+2-2S)}{2y(y+2)S(2S+1)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S-1)(y+2+2S)(y+4+2S)}{4(y+1)(y+2)(2S+1)}\right]^{\frac{1}{2}}$
$S\ S;\ 11$	SS	$\frac{\{y+2-2S(S+1)\}}{[2y(y+2)S(S+1)]^{\frac{1}{2}}}$	$\left[\frac{(y+2-2S)(y+4+2S)}{4(y+1)(y+2)}\right]^{\frac{1}{2}}$
$S\ S;\ 00$	SS	$-\left[\frac{2S(S+1)}{y(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+2-2S)(y+4+2S)}{4(y+1)(y+2)}\right]^{\frac{1}{2}}$
$S\ S;\ 11$	$S(S-1)$	$\left[\frac{(S+1)(y+2-2S)}{2yS}\right]^{\frac{1}{2}}$	
$S\ S;\ 11$	$(S-1)S$		
$S-1\ S-1;\ 11$	$S(S-1)$	$\left[\frac{(S-1)(y+2+2S)}{2yS}\right]^{\frac{1}{2}}$	
$S-1\ S-1;\ 11$	$(S-1)S$		

TABLE A3.4.

$S_1T_1;\ S_2T_2$	ST	$\left\langle \begin{matrix}[y-1\ 10]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y+1\ 10] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[y-1\ 10]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y11] \\ ST\end{matrix} \right\rangle$
$S+1\ S+1;\ 11$	SS	$\frac{1}{2(S+1)}\left[\frac{S(S+2)(2S+3)(y-2-2S)(y-2S)}{y(y-1)(2S+1)}\right]^{\frac{1}{2}}$	0
$S+1\ S;\ 11$	SS	$\frac{1}{2(S+1)}\left[\frac{(2S+3)(y-2S)}{(y-1)(2S+1)}\right]^{\frac{1}{2}}$	$\pm\left[\frac{(2S+3)(y-2S)}{4(y-1)(2S+1)}\right]^{\frac{1}{2}}$
$S\ S+1;\ 11$	SS		
$S\ S;\ 11$	SS	$\frac{\{S^2+S-1\}}{2S(S+1)}\left[\frac{(y-2S)(y+2+2S)}{y(y-1)}\right]^{\frac{1}{2}}$	0
$S\ S-1;\ 11$	SS	$\frac{1}{2S}\left[\frac{(2S-1)(y+2+2S)}{(y-1)(2S+1)}\right]^{\frac{1}{2}}$	$\pm\left[\frac{(2S-1)(y+2+2S)}{4(y-1)(2S+1)}\right]^{\frac{1}{2}}$
$S-1\ S;\ 11$	SS		
$S-1\ S-1;\ 11$	SS	$\frac{1}{2S}\left[\frac{(S-1)(S+1)(2S-1)(y+2+2S)(y+2S)}{y(y-1)(2S+1)}\right]^{\frac{1}{2}}$	0
$S\ S;\ 00$	SS	$\left[\frac{(y-2S)(y+2+2S)}{4y(y-1)}\right]^{\frac{1}{2}}$	0
$S+1\ S;\ 11$	$S\ S-1$	$\left[\frac{(2S+3)(y-2S)(y+2-2S)}{4(y-1)(y+2)(2S+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S+3)(y-2S)(y+2+2S)}{4(y-1)(y+2)(2S+1)}\right]^{\frac{1}{2}}$
$S\ S;\ 11$	$S\ S-1$	$\frac{-1}{2S}\left[\frac{(y-2S)(y+2+2S)(y+2-2S)}{y(y-1)(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{y(y-2S)}{4(y-1)(y+2)}\right]^{\frac{1}{2}}$
$S\ S-1;\ 11$	$S\ S-1$	$\frac{1}{2S}\left[\frac{(S-1)(S+1)(y+2+2S)(y+2-2S)}{(y-1)(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{(S-1)(S+1)}{(y-1)(y+2)}\right]^{\frac{1}{2}}$
$S-1\ S;\ 11$	$S\ S-1$	$\frac{-1}{2S}\left[\frac{(y+2+2S)(y+2-2S)}{(y-1)(y+2)(2S+1)(2S-1)}\right]^{\frac{1}{2}}$	$\frac{-(y+1)}{[(y-1)(y+2)(2S-1)(2S+1)]^{\frac{1}{2}}}$
$S-1\ S-1;\ 11$	$S\ S-1$	$\frac{-1}{2S}\left[\frac{(y+2S)(y+2+2S)(y+2-2S)}{y(y-1)(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{y(y+2S)}{4(y-1)(y+2)}\right]^{\frac{1}{2}}$
$S-1\ S-2;\ 11$	$S\ S-1$	$\left[\frac{(2S-3)(y+2S)(y+2+2S)}{4(2S-1)(y-1)(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S-3)(y+2S)(y+2-2S)}{4(2S-1)(y-1)(y+2)}\right]^{\frac{1}{2}}$
$S\ S-1;\ 00$	$S\ S-1$	$\left[\frac{(y+2+2S)(y+2-2S)}{4(y-1)(y+2)}\right]^{\frac{1}{2}}$	$\frac{-S}{[(y-1)(y+2)]^{\frac{1}{2}}}$

$$\left\langle \begin{matrix}[y-1\ 10]\ [200] \\ T_1S_1;\ T_2S_2\end{matrix} \middle\| \begin{matrix}[y+1\ 10] \\ (S-1)S\end{matrix} \right\rangle = +\left\langle \begin{matrix}[y-1\ 10]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y+1\ 10] \\ S(S-1)\end{matrix} \right\rangle;$$

$$\left\langle \begin{matrix}[y-1\ 10]\ [200] \\ T_1S_1;\ T_2S_2\end{matrix} \middle\| \begin{matrix}[y11] \\ (S-1)S\end{matrix} \right\rangle = -\left\langle \begin{matrix}[y-1\ 10]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y11] \\ S(S-1)\end{matrix} \right\rangle.$$

TABLE A3.5.

$S_1T_1;\ S_2T_2$	ST	$\left\langle \begin{matrix}[y11]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y+2\ 11] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[y11]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y-1\ 10] \\ ST\end{matrix} \right\rangle$	$\left\langle \begin{matrix}[y11]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y00] \\ SS\end{matrix} \right\rangle$
$S+1\ S+1;\ 11$	SS	$\left[\frac{S(S+2)(2S+3)(y+2-2S)(y-2S)(y+2)}{4y(y+1)(y+4)(2S+1)(S+1)^2}\right]^{\frac{1}{2}}$	$-\left[\frac{S(S+2)(2S+3)(y+2+2S)(y+4+2S)}{8y(y+3)(2S+1)(S+1)^2}\right]^{\frac{1}{2}}$	$\left[\frac{(S+2)(2S+3)(y-2S)(y+4+2S)}{6y(y+4)(S+1)(2S+1)}\right]^{\frac{1}{2}}$
$S+1\ S;\ 11$	SS	$-\left[\frac{(2S+3)(y-2S)(y+2-2S)(y+4+2S)}{4y(y+1)(y+4)(2S+1)(S+1)^2}\right]^{\frac{1}{2}}$	$-\left[\frac{S^2(2S+3)(y+2+2S)(y+2)}{8y(y+3)(2S+1)(S+1)^2}\right]^{\frac{1}{2}}$	$\left[\frac{S(2S+3)(y-2S)(y+2)}{6y(y+4)(S+1)(2S+1)}\right]^{\frac{1}{2}}$
$S\ S+1;\ 11$	SS			
$S\ S;\ 11$	SS	$\frac{\{S(S+1)-1\}}{2S(S+1)}\left[\frac{(y+2-2S)(y+4+2S)(y+2)}{y(y+1)(y+4)}\right]^{\frac{1}{2}}$	$\frac{\{S(S+1)+1\}}{2S(S+1)}\left[\frac{(y-2S)(y+2+2S)}{2y(y+3)}\right]^{\frac{1}{2}}$	$\frac{\{2S(S+1)+(y+2)\}}{[6y(y+4)S(S+1)]^{\frac{1}{2}}}$
$S\ S-1;\ 11$	SS	$-\left[\frac{(2S-1)(y+2-2S)(y+2+2S)(y+4+2S)}{4y(y+1)(y+4)(2S+1)S^2}\right]^{\frac{1}{2}}$	$\left[\frac{(S+1)^2(2S-1)(y-2S)(y+2)}{8y(y+3)(2S+1)S^2}\right]^{\frac{1}{2}}$	$\left[\frac{(S+1)(2S-1)(y+2+2S)(y+2)}{6y(y+4)S(2S+1)}\right]^{\frac{1}{2}}$
$S-1\ S;\ 11$	SS			
$S-1\ S-1;\ 11$	SS	$\left[\frac{(S-1)(S+1)(2S-1)(y+2+2S)(y+4+2S)(y+2)}{4y(y+1)(y+4)(2S+1)S^2}\right]^{\frac{1}{2}}$	$-\left[\frac{(S-1)(S+1)(2S-1)(y+2-2S)(y-2S)}{8y(y+3)(2S+1)S^2}\right]^{\frac{1}{2}}$	$-\left[\frac{(S-1)(2S-1)(y+2+2S)(y+2-2S)}{6y(y+4)S(2S+1)}\right]^{\frac{1}{2}}$
$S\ S;\ 00$	SS	$\left[\frac{(y+2-2S)(y+4+2S)(y+2)}{4y(y+1)(y+4)}\right]^{\frac{1}{2}}$	$\left[\frac{(y-2S)(y+2+2S)}{8y(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{2S(S+1)}{3y(y+4)}\right]^{\frac{1}{2}}$
$S+1\ S;\ 11$	$S(S-1)$	$\left[\frac{(2S+3)(y+2-2S)(y-2S)}{4y(y+1)(2S+1)}\right]^{\frac{1}{2}}$	0	
$S\ S;\ 11$	$S(S-1)$	$\frac{1}{2S}\left[\frac{(y+2)(y+2-2S)}{y(y+1)}\right]^{\frac{1}{2}}$	$\frac{(S+1)}{2S}\left[\frac{(y+2+2S)}{2(y+3)}\right]^{\frac{1}{2}}$	
$S\ S-1;\ 11$	$S(S-1)$	$\frac{1}{2S}\left[\frac{(S+1)(S-1)(y+2+2S)(y+2-2S)}{y(y+1)}\right]^{\frac{1}{2}}$	$\frac{1}{2S}\left[\frac{(S+1)(S-1)(y+2)}{2(y+3)}\right]^{\frac{1}{2}}$	
$S-1\ S;\ 11$	$S(S-1)$	$\frac{-1}{2S}\left[\frac{(y+2+2S)(y+2-2S)}{y(y+1)(2S-1)(2S+1)}\right]^{\frac{1}{2}}$	$\frac{1}{2S}\left[\frac{(2S-1)(2S+1)(y+2)}{2(y+3)}\right]^{\frac{1}{2}}$	
$S-1\ S-1;\ 11$	$S(S-1)$	$\frac{1}{2S}\left[\frac{(y+2)(y+2+2S)}{y(y+1)}\right]^{\frac{1}{2}}$	$-\frac{(S-1)}{2S}\left[\frac{(y+2-2S)}{2(y+3)}\right]^{\frac{1}{2}}$	
$S-1\ S-2;\ 11$	$S(S-1)$	$\left[\frac{(2S-3)(y+2+2S)(y+2S)}{4y(y+1)(2S-1)}\right]^{\frac{1}{2}}$	0	
$S\ S-1;\ 00$	$S(S-1)$	$\left[\frac{(y+2+2S)(y+2-2S)}{4y(y+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(y+2)}{8(y+3)}\right]^{\frac{1}{2}}$	

$$\left\langle \begin{matrix}[y11]\ [200] \\ T_1S_1;\ T_2S_2\end{matrix} \middle\| \begin{matrix}[f'] \\ (S-1)S\end{matrix} \right\rangle = \left\langle \begin{matrix}[y11]\ [200] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[f'] \\ S(S-1)\end{matrix} \right\rangle \quad \text{for both} \quad \begin{matrix}[f']=[y+2\ 11], \\ [f']=[y-1\ 10].\end{matrix}$$

TABLE A4.1.

$S_1T_1;\quad S_2T_2$	$\left\langle \begin{matrix}[yy0]\ [211] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| [yy0]\ ST \right\rangle$
$S+1\ T+1;\ 11$	$-\left[\frac{(S+1)(T+1)(y-S-T)(y+S+T+4)}{(2S+1)(2T+1)y(y+4)}\right]^{\frac{1}{2}}$
$S+1\ T-1;\ 11$	$\left[\frac{(S+1)T(y-S+T+1)(y+S-T+3)}{(2S+1)(2T+1)y(y+4)}\right]^{\frac{1}{2}}$
$S-1\ T+1;\ 11$	$\left[\frac{S(T+1)(y+S-T+1)(y-S+T+3)}{(2S+1)(2T+1)y(y+4)}\right]^{\frac{1}{2}}$
$S-1\ T-1;\ 11$	$-\left[\frac{ST(y-S-T+2)(y+S+T+2)}{(2S+1)(2T+1)y(y+4)}\right]^{\frac{1}{2}}$
$S\ T;\quad 10$	$\left[\frac{S(S+1)}{y(y+4)}\right]^{\frac{1}{2}}$
$S\ T;\quad 01$	$\left[\frac{T(T+1)}{y(y+4)}\right]^{\frac{1}{2}}$

TABLE A4.2.

$S_1T_1;\quad S_2T_2$	$\left\langle \begin{matrix}[y00]\ [211] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| [y00]\ ST \right\rangle$
$S+1\ S+1;\ 11$	$-\left[\frac{(2S+3)(y-2S)(y+4+2S)}{(2S+1)3y(y+4)}\right]^{\frac{1}{2}}$
$S\ S;\quad 11$	$\frac{-(y+2)}{[3y(y+4)]^{\frac{1}{2}}}$
$S-1\ S-1;\ 11$	$-\left[\frac{(2S-1)(y+2-2S)(y+2+2S)}{(2S+1)3y(y+4)}\right]^{\frac{1}{2}}$
$S\ S;\quad 10$	$\left[\frac{4S(S+1)}{3y(y+4)}\right]^{\frac{1}{2}}$
$S\ S;\quad 01$	

TABLE A4.3.

$$\left\langle \begin{matrix} [y\ y-1\ 0]\ [211] \\ S_1T_1;\ S_2T_2 \end{matrix} \middle\| \begin{matrix} [y\ y-1\ 0] \\ ST \end{matrix} \right\rangle$$

$S_1T_1;\ S_2T_2$	$\rho = 1$	$\rho = 2$
	(a) $y - S - T$ = even integer	
$S+1\ T+1;\ 11$	$-\left[\frac{(2S+3)(2T+3)(y-S-T)(y+S+T+4)}{4(S+1)(T+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\frac{(y+2)(2y-7)[(2S+3)(2T+3)(y-S-T)(y+S+T+4)]^{\frac{1}{2}}}{4[6(S+1)(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S+1\ T;\ 11$	$-\left[\frac{(2S+3)(y-S-T)(y+S-T+2)}{4(S+1)T(T+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{\{(2y+13)(y+1)+T(4y^2+12y-1)\}[(2S+3)(y-S-T)(y+S-T+2)]^{\frac{1}{2}}}{4[6(S+1)T(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S+1\ T-1;\ 11$	$\left[\frac{(2S+3)(2T-1)(y-S+T)(y+S-T+2)}{4(S+1)T(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\frac{(2y+13)(y+1)[(2S+3)(2T-1)(y-S+T)(y+S-T+2)]^{\frac{1}{2}}}{4[6(S+1)T(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S\ T+1;\ 11$	$-\left[\frac{(2T+3)(y-S-T)(y-S+T+2)}{4S(S+1)(T+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{\{(2y+13)(y+1)+S(4y^2+12y-1)\}[(2T+3)(y-S-T)(y-S+T+2)]^{\frac{1}{2}}}{4[6S(S+1)(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S\ T;\ 11$	$-\frac{\{(y+\frac{3}{2})+2(S+\frac{1}{2})(T+\frac{1}{2})\}}{[4S(S+1)T(T+1)(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{\left\{\frac{1}{2}(16y^2+48y+41)-[S(S+1)+T(T+1)](4y^2+12y-1)\right.}{4[6S(S+1)T(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$ $\left.-2(S+\frac{1}{2})(T+\frac{1}{2})(2y+3)(2y^2+6y-5)\right\}$
$S\ T-1;\ 11$	$\left[\frac{(2T-1)(y+S-T+2)(y+S+T+2)}{4S(S+1)T(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{\{(2y-7)(y+2)+S(4y^2+12y-1)\}[(2T-1)(y+S-T+2)(y+S+T+2)]^{\frac{1}{2}}}{4[6ST(S+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S-1\ T+1;\ 11$	$\left[\frac{(2S-1)(2T+3)(y+S-T)(y-S+T+2)}{4S(T+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\frac{(2y+13)(y+1)[(2S-1)(2T+3)(y+S-T)(y-S+T+2)]^{\frac{1}{2}}}{4[6S(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S-1\ T;\ 11$	$\left[\frac{(2S-1)(y+S+T+2)(y-S+T+2)}{4ST(T+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{\{(2y-7)(y+2)+T(4y^2+12y-1)[(2S-1)(y+S+T+2)(y-S+T+2)]^{\frac{1}{2}}}{4[6ST(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S-1\ T-1;\ 11$	$-\left[\frac{(2S-1)(2T-1)(y-S-T+2)(y+S+T+2)}{4ST(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\frac{(y+2)(2y-7)[(2S-1)(2T-1)(y-S-T+2)(y+S+T+2)]^{\frac{1}{2}}}{4[6ST(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S+1\ T;\ 10$	0	$\frac{[(2S+3)(y-S-T)(y+S-T+2)(4y^2+12y-1)]^{\frac{1}{2}}}{4[6(S+1)(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}}$
$S\ T;\ 10$	$\left[\frac{4S(S+1)}{(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{\{[(4y^2+12y-1)][(2y+3)+(2S+1)(2T+1)]-36(2y+3)S(S+1)\}}{8[6S(S+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S-1\ T;\ 10$	0	$-\frac{[(2S-1)(y+S+T+2)(y-S+T+2)(4y^2+12y-1)]^{\frac{1}{2}}}{4[6S(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}}$
$S\ T+1;\ 01$	0	$\frac{[(2T+3)(y-S-T)(y-S+T+2)(4y^2+12y-1)]^{\frac{1}{2}}}{4[6(T+1)(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}}$
$S\ T;\ 01$	$\left[\frac{4T(T+1)}{(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{\{[(4y^2+12y-1)][(2y+3)+(2S+1)(2T+1)]-36(2y+3)T(T+1)\}}{8[6T(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S\ T-1;\ 01$	0	$-\frac{[(2T-1)(y+S+T+2)(y+S-T+2)(4y^2+12y-1)]^{\frac{1}{2}}}{4[6T(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}}$

(b) $y - S - T =$ odd integer

$S+1\ T+1;$	11	$-\left[\frac{(2S+3)(2T+3)(y-S-T-1)(y+S+T+3)}{4(S+1)(T+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{(2y+13)(y+1)[(2S+3)(2T+3)(y-S-T-1)(y+S+T+3)]^{\frac{1}{2}}}{4[6(S+1)(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S+1\ T;$	11	$-\left[\frac{(2S+3)(y-S+T+1)(y+S+T+3)}{4(S+1)T(T+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\frac{\{(2y-7)(y+2)+T(4y^2+12y-1)\}[(2S+3)(y-S+T+1)(y+S+T+3)]^{\frac{1}{2}}}{4[6(S+1)T(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S+1\ T-1;$	11	$\left[\frac{(2S+3)(2T-1)(y+S-T+3)(y-S+T+1)}{4(S+1)T(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{(2y-7)(y+2)[(2S+3)(2T-1)(y+S-T+3)(y-S+T+1)]^{\frac{1}{2}}}{4[6(S+1)T(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S\ T+1;$	11	$-\left[\frac{(2T+3)(y+S-T+1)(y+S+T+3)}{4S(S+1)(T+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\frac{\{(2y-7)(y+2)+S(4y^2+12y-1)\}[(2T+3)(y+S-T+1)(y+S+T+3)]^{\frac{1}{2}}}{4[6S(S+1)(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S\ T;$	11	$-\frac{\{(y+\frac{3}{2})-2(S+\frac{1}{2})(T+\frac{1}{2})\}}{[4S(S+1)T(T+1)(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{\left\{\begin{array}{r}\frac{1}{2}(16y^2+48y+41)-[S(S+1)+T(T+1)](4y^2+12y-1)\\ +2(S+\frac{1}{2})(T+\frac{1}{2})(2y+3)(2y^2+6y-5)\end{array}\right\}}{4[6S(S+1)T(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S\ T-1;$	11	$\left[\frac{(2T-1)(y-S-T+1)(y-S+T+1)}{4S(S+1)T(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\frac{\{(2y+13)(y+1)+S(4y^2+12y-1)\}[(2T-1)(y-S+T+1)(y-S-T+1)]^{\frac{1}{2}}}{4[6ST(S+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S-1\ T+1;$	11	$\left[\frac{(2S-1)(2T+3)(y+S-T+1)(y-S+T+3)}{4S(T+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{(2y-7)(y+2)[(2S-1)(2T+3)(y+S-T+1)(y-S+T+3)]^{\frac{1}{2}}}{4[6S(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S-1\ T;$	11	$\left[\frac{(2S-1)(y-S-T+1)(y+S-T+1)}{4ST(T+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\frac{\{(2y+13)(y+1)+T(4y^2+12y-1)\}[(2S-1)(y+S-T+1)(y-S-T+1)]^{\frac{1}{2}}}{4[6ST(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S-1\ T-1;$	11	$-\left[\frac{(2S-1)(2T-1)(y-S-T+1)(y+S+T+1)}{4ST(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{(2y+13)(y+1)[(2S-1)(2T-1)(y+S+T+1)(y-S-T+1)]^{\frac{1}{2}}}{4[6ST(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S+1\ T;$	10	0	$\frac{[(2S+3)(y-S+T+1)(y+S+T+3)(4y^2+12y-1)]^{\frac{1}{2}}}{4[6(S+1)(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}}$
$S\ T;$	10	$\left[\frac{4S(S+1)}{(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{\{[(4y^2+12y-1)][(2y+3)-(2S+1)(2T+1)]-36(2y+3)S(S+1)\}}{8[6S(S+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S-1\ T;$	10	0	$-\frac{[(2S-1)(y+S-T+1)(y-S-T+1)(4y^2+12y-1)]^{\frac{1}{2}}}{4[6S(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}}$
$S\ T+1;$	01	0	$\frac{[(2T+3)(y+S-T+1)(y+S+T+3)(4y^2+12y-1)]^{\frac{1}{2}}}{4[6(T+1)(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}}$
$S\ T;$	01	$\left[\frac{4T(T+1)}{(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{\{[(4y^2+12y-1)][(2y+3)-(2S+1)(2T+1)]-36(2y+3)T(T+1)\}}{8[6T(T+1)(y-1)(y+1)(y+2)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$
$S\ T-1;$	01	0	$-\frac{[(2T-1)(y-S+T+1)(y-S-T+1)(4y^2+12y-1)]^{\frac{1}{2}}}{4[6T(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}}$

TABLE A4.4.

$$\left\langle \begin{matrix} [y\ y-1\ 0]\ [211] \\ S_1T_1;\ S_2T_2 \end{matrix} \middle\| \begin{matrix} [y+1\ y+1\ 1] \\ ST \end{matrix} \right\rangle$$

$S_1T_1;\ S_2T_2$	$y-S-T=$ odd integer	$y-S-T=$ even integer
$S+1\ T+1;\ 11$	$\left[\frac{(2S+3)(2T+3)(y-S-T+1)(y-S-T-1)}{32(S+1)(T+1)y(y+2)}\right]^{\frac{1}{2}}$	0
$S+1\ T;\ 11$	$-\left[\frac{(2S+3)T(y-S-T+1)(y-S+T+1)}{32(S+1)(T+1)y(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S+3)(T+1)(y-S-T)(y-S+T+2)}{32(S+1)Ty(y+2)}\right]^{\frac{1}{2}}$
$S+1\ T-1;\ 11$	0	$-\left[\frac{(2S+3)(2T-1)(y-S+T)(y-S+T+2)}{32(S+1)Ty(y+2)}\right]^{\frac{1}{2}}$
$S\ T+1;\ 11$	$-\left[\frac{S(2T+3)(y-S-T+1)(y+S-T+1)}{32(S+1)(T+1)y(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{(S+1)(2T+3)(y-S-T)(y+S-T+2)}{32S(T+1)y(y+2)}\right]^{\frac{1}{2}}$
$S\ T;\ 11$	$-(S+T+1)\left[\frac{(y+S+T+3)(y-S-T+1)}{32S(S+1)T(T+1)y(y+2)}\right]^{\frac{1}{2}}$	$-(S-T)\left[\frac{(y+S-T+2)(y-S+T+2)}{32S(S+1)T(T+1)y(y+2)}\right]^{\frac{1}{2}}$
$S\ T-1;\ 11$	$\left[\frac{(S+1)(2T-1)(y-S+T+1)(y+S+T+3)}{32STy(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{S(2T-1)(y+S+T+2)(y-S+T+2)}{32(S+1)Ty(y+2)}\right]^{\frac{1}{2}}$
$S-1\ T+1;\ 11$	0	$\left[\frac{(2S-1)(2T+3)(y+S-T)(y+S-T+2)}{32S(T+1)y(y+2)}\right]^{\frac{1}{2}}$
$S-1\ T;\ 11$	$\left[\frac{(2S-1)(T+1)(y+S+T+3)(y+S-T+1)}{32STy(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2S-1)T(y+S+T+2)(y+S-T+2)}{32S(T+1)y(y+2)}\right]^{\frac{1}{2}}$
$S-1\ T\ 0;-11$	$-\left[\frac{(2S-1)(2T-1)(y+S+T+1)(y+S+T+3)}{32STy(y+2)}\right]^{\frac{1}{2}}$	0
$S+1\ T;\ 10$	$\left[\frac{(2S+3)(y-S-T+1)(y-S+T+1)}{32(S+1)y(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S+3)(y-S-T)(y-S+T+2)}{32(S+1)y(y+2)}\right]^{\frac{1}{2}}$
$ST;\ 10$	$-(2S+1)\left[\frac{(y-S-T+1)(y+S+T+3)}{32S(S+1)y(y+2)}\right]^{\frac{1}{2}}$	$-(2S+1)\left[\frac{(y+S-T+2)(y-S+T+2)}{32S(S+1)y(y+2)}\right]^{\frac{1}{2}}$
$S-1\ T;\ 10$	$\left[\frac{(2S-1)(y+S-T+1)(y+S+T+3)}{32Sy(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(2S-1)(y+S+T+2)(y+S-T+2)}{32Sy(y+2)}\right]^{\frac{1}{2}}$
$S\ T+1;\ 01$	$\left[\frac{(2T+3)(y-S-T+1)(y+S-T+1)}{32(T+1)y(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2T+3)(y-S-T)(y+S-T+2)}{32(T+1)y(y+2)}\right]^{\frac{1}{2}}$
$S\ T;\ 01$	$-(2T+1)\left[\frac{(y-S-T+1)(y+S+T+3)}{32T(T+1)y(y+2)}\right]^{\frac{1}{2}}$	$(2T+1)\left[\frac{(y-S+T+2)(y+S-T+2)}{32T(T+1)y(y+2)}\right]^{\frac{1}{2}}$
$S\ T-1;\ 01$	$\left[\frac{(2T-1)(y-S+T+1)(y+S+T+3)}{32Ty(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{(2T-1)(y+S+T+2)(y-S+T+2)}{32Ty(y+2)}\right]^{\frac{1}{2}}$

TABLE A4.5. $\left\langle \begin{matrix}[y10]\ [211] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y10] \\ ST\end{matrix} \right\rangle_\rho$.

$S_1T_1;\ S_2T_2$	ST	$\rho = 1$	$\rho = 2$
$S+1\ S+1;\ 11$	SS	$-\left[\frac{S(S+2)(2S+3)(y-1-2S)(y+3+2S)}{(2S+1)(S+1)^2(y+1)(3y+7)}\right]^{\frac{1}{2}}$	$-\frac{(y+9)}{2(S+1)}\left[\frac{S(S+2)(2S+3)(y-1-2S)(y+3+2S)}{2(2S+1)(y-1)(y+4)(y+1)(3y+7)}\right]^{\frac{1}{2}}$
$S+1\ S;\ 11$	SS	$\frac{-1}{(S+1)}\left[\frac{(2S+3)(y+3+2S)}{(2S+1)(3y+7)}\right]^{\frac{1}{2}}$	$\frac{\{(y-11)+S(3y+7)\}}{4(S+1)}\left[\frac{(2S+3)(y+3+2S)}{2(2S+1)(y-1)(y+4)(3y+7)}\right]^{\frac{1}{2}}$
$S\ S+1;\ 11$	SS		
$S\ S;\ 11$	SS	$\frac{\{(y+1)-(y+3)S(S+1)\}}{S(S+1)[(y+1)(3y+7)]^{\frac{1}{2}}}$	$\frac{\{(y+1)(y+9)+2(y^2-y-10)S(S+1)\}}{2S(S+1)[2(y-1)(y+4)(y+1)(3y+7)]^{\frac{1}{2}}}$
$S\ S-1;\ 11$	SS	$\frac{-1}{S}\left[\frac{(2S-1)(y+1-2S)}{(2S+1)(3y+7)}\right]^{\frac{1}{2}}$	$\frac{-\{2(y+9)+S(3y+7)\}}{4S}\left[\frac{(2S-1)(y+1-2S)}{2(2S+1)(y-1)(y+4)(3y+7)}\right]^{\frac{1}{2}}$
$S-1\ S;\ 11$	SS		
$S-1\ S-1;\ 11$	SS	$\frac{-1}{S}\left[\frac{(S-1)(S+1)(2S-1)(y+1+2S)(y+1-2S)}{(2S+1)(y+1)(3y+7)}\right]^{\frac{1}{2}}$	$-\frac{(y+9)}{2S}\left[\frac{(S-1)(S+1)(2S-1)(y+1+2S)(y+1-2S)}{2(2S+1)(y-1)(y+4)(y+1)(3y+7)}\right]^{\frac{1}{2}}$
$S+1\ S;\ 10$	SS	0	$\left[\frac{S(2S+3)(y+3+2S)(3y+7)}{32(S+1)(2S+1)(y-1)(y+4)}\right]^{\frac{1}{2}}$
$S\ S+1;\ 01$	SS		
$S-1\ S;\ 10$	SS	0	$\left[\frac{(S+1)(2S-1)(y+1-2S)(3y+7)}{32S(2S+1)(y-1)(y+4)}\right]^{\frac{1}{2}}$
$S\ S-1;\ 01$	SS		
$S\ S;\ 10$	SS	$\left[\frac{4S(S+1)}{(y+1)(3y+7)}\right]^{\frac{1}{2}}$	$-\frac{\{(y+1)(3y+7)-4(y+9)S(S+1)\}}{4[2S(S+1)(y-1)(y+4)(y+1)(3y+7)]^{\frac{1}{2}}}$
$S\ S;\ 01$	SS		
$S+1\ S;\ 11$	$S\ S-1$	$-\left[\frac{(2S+3)(y+3+2S)(y+1-2S)}{(2S+1)(y+1)(3y+7)}\right]^{\frac{1}{2}}$	$(y-11)\left[\frac{(2S+3)(y+3+2S)(y+1-2S)}{32(2S+1)(y-1)(y+4)(y+1)(3y+7)}\right]^{\frac{1}{2}}$
$S\ S;\ 11$	$S\ S-1$	$\frac{1}{S}\left[\frac{y+1-2S}{(3y+7)}\right]^{\frac{1}{2}}$	$\frac{\{2(y+9)+S(3y+7)\}}{4S}\left[\frac{(y+1-2S)}{2(y-1)(y+4)(3y+7)}\right]^{\frac{1}{2}}$
$S\ S-1;\ 11$	$S\ S-1$	$-\frac{1}{S}\left[\frac{(S-1)(S+1)(y+1)}{(3y+7)}\right]^{\frac{1}{2}}$	$-\frac{(y+9)}{2S}\left[\frac{(S-1)(S+1)(y+1)}{2(y-1)(y+4)(3y+7)}\right]^{\frac{1}{2}}$
$S-1\ S;\ 11$	$S\ S-1$	$\frac{\{y+1+4S^2\}}{S[(2S-1)(2S+1)(y+1)(3y+7)]}$	$\frac{\{(y+1)(y+9)-2S^2(3y-1)(y+4)\}}{2S[2(2S-1)(2S+1)(y-1)(y+4)(y+1)(3y+7)]^{\frac{1}{2}}}$
$S-1\ S-1;\ 11$	$S\ S-1$	$\frac{1}{S}\left[\frac{y+1+2S}{3y+7}\right]^{\frac{1}{2}}$	$\frac{\{2(y+9)-S(3y+7)\}}{4S}\left[\frac{(y+1+2S)}{2(y-1)(y+4)(3y+7)}\right]^{\frac{1}{2}}$
$S-1\ S-2;\ 11$	$S\ S-1$	$-\left[\frac{(2S-3)(y+3-2S)(y+1+2S)}{(2S-1)(y+1)(3y+7)}\right]^{\frac{1}{2}}$	$(y-11)\left[\frac{(2S-3)(y+3-2S)(y+1+2S)}{32(2S-1)(y-1)(y+4)(y+1)(3y+7)}\right]^{\frac{1}{2}}$
$S\ S-1;\ 10$	$S\ S-1$	$\left[\frac{4S(S+1)}{(y+1)(3y+7)}\right]^{\frac{1}{2}}$	$-\frac{\{(y+1)(3y+7)+2(y-11)S\}(S+1)}{4[2S(S+1)(y-1)(y+4)(y+1)(3y+7)]^{\frac{1}{2}}}$
$S-1\ S-1;\ 10$	$S\ S-1$	0	$-\left[\frac{(S-1)(y+1+2S)(3y+7)}{32S(y-1)(y+4)}\right]^{\frac{1}{2}}$
$S\ S;\ 10$	$S\ S-1$	0	$-\left[\frac{(S+1)(y+1-2S)(3y+7)}{32S(y-1)(y+4)}\right]^{\frac{1}{2}}$
$S\ S-1;\ 01$	$S\ S-1$	$\left[\frac{4(S-1)S}{(y+1)(3y+7)}\right]^{\frac{1}{2}}$	$\frac{\{(y+1)(3y+7)-2(y-11)S\}(S-1)}{4[2(S-1)S(y-1)(y+4)(y+1)(3y+7)]^{\frac{1}{2}}}$

$$\left\langle \begin{matrix}[y10]\ [211] \\ T_1S_1;\ T_2S_2\end{matrix} \middle\| \begin{matrix}[y10] \\ (S-1)S\end{matrix} \right\rangle_\rho = \left\langle \begin{matrix}[y10]\ [211] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y10] \\ S(S-1)\end{matrix} \right\rangle_\rho .$$

TABLE A4.6. $\left\langle \begin{matrix}[y11]\ [211] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y11] \\ ST\end{matrix} \right\rangle_\rho$.

$S_1T_1;\ S_2T_2$	ST	$\rho = 1$	$\rho = 2$
$S+1\ S+1;\ 11$	SS	$-\left[\frac{S(2S+3)(S+2)(y-2S)(y+4+2S)}{(2S+1)(S+1)^2(y+2)(3y+2)}\right]^{\frac{1}{2}}$	$-\frac{(y-6)}{2(S+1)}\left[\frac{S(S+2)(2S+3)(y-2S)(y+4+2S)}{2(2S+1)(y-1)(y+4)(y+2)(3y+2)}\right]^{\frac{1}{2}}$
$S+1\ S;\ 11$	SS	$\frac{1}{(S+1)}\left[\frac{(2S+3)(y-2S)}{(2S+1)(3y+2)}\right]^{\frac{1}{2}}$	$\frac{\{2(y-6)-(S+1)(3y+2)\}}{4(S+1)}\left[\frac{(2S+3)(y-2S)}{2(2S+1)(y-1)(y+4)(3y+2)}\right]^{\frac{1}{2}}$
$S\ S+1;\ 11$	SS		
$S\ S;\ 11$	SS	$\frac{\{(y+2)-yS(S+1)\}}{S(S+1)[(y+2)(3y+2)]^{\frac{1}{2}}}$	$\frac{\{(y+2)(y-6)+2(y^2+7y+2)S(S+1)\}}{2S(S+1)[2(y-1)(y+4)(y+2)(3y+2)]^{\frac{1}{2}}}$
$S\ S-1;\ 11$	SS	$\frac{1}{S}\left[\frac{(2S-1)(y+2+2S)}{(2S+1)(3y+2)}\right]^{\frac{1}{2}}$	$\frac{\{2(y-6)+S(3y+2)\}}{4S}\left[\frac{(2S-1)(y+2+2S)}{2(2S+1)(y-1)(y+4)(3y+2)}\right]^{\frac{1}{2}}$
$S-1\ S;\ 11$	SS		
$S-1\ S-1;\ 11$	SS	$-\frac{1}{S}\left[\frac{(S-1)(S+1)(2S-1)(y+2+2S)(y+2-2S)}{(2S+1)(y+2)(3y+2)}\right]^{\frac{1}{2}}$	$-\frac{(y-6)}{2S}\left[\frac{(S-1)(S+1)(2S-1)(y+2+2S)(y+2-2S)}{2(2S+1)(y-1)(y+4)(y+2)(3y+2)}\right]^{\frac{1}{2}}$
$S+1\ S;\ 10$	SS		$\left[\frac{S(2S+3)(y-2S)(3y+2)}{32(S+1)(2S+1)(y-1)(y+4)}\right]^{\frac{1}{2}}$
$S\ S+1;\ 01$	SS	0	
$S\ S;\ 10$	SS	$\left[\frac{4S(S+1)}{(y+2)(3y+2)}\right]^{\frac{1}{2}}$	$\frac{\{(y+2)(3y+2)+4(y-6)S(S+1)\}}{4[2S(S+1)(y-1)(y+4)(y+2)(3y+2)]^{\frac{1}{2}}}$
$S\ S;\ 01$	SS		
$S-1\ S;\ 10$	SS		$\left[\frac{(S+1)(2S-1)(y+2+2S)(3y+2)}{32S(2S+1)(y-1)(y+4)}\right]^{\frac{1}{2}}$
$S\ S-1;\ 01$	SS	0	
$S+1\ S;\ 11$	$S\ S-1$	$-\left[\frac{(2S+3)(y-2S)(y+2+2S)}{(2S+1)(y+2)(3y+2)}\right]^{\frac{1}{2}}$	$\frac{(y+14)}{4}\left[\frac{(2S+3)(y-2S)(y+2+2S)}{2(2S+1)(y-1)(y+4)(y+2)(3y+2)}\right]^{\frac{1}{2}}$
$S\ S;\ 11$	$S\ S-1$	$-\frac{1}{S}\left[\frac{(y+2+2S)}{(3y+2)}\right]^{\frac{1}{2}}$	$-\frac{\{2(y-6)+S(3y+2)\}}{4S}\left[\frac{(y+2+2S)}{2(y-1)(y+4)(3y+2)}\right]^{\frac{1}{2}}$
$S\ S-1;\ 11$	$S\ S-1$	$-\frac{1}{S}\left[\frac{(S-1)(S+1)(y+2)}{(3y+2)}\right]^{\frac{1}{2}}$	$-\frac{(y-6)}{2S}\left[\frac{(S-1)(S+1)(y+2)}{2(y-1)(y+4)(3y+2)}\right]^{\frac{1}{2}}$
$S-1\ S;\ 11$	$S\ S-1$	$\frac{\{(y+2)-4S^2\}}{S[(2S-1)(2S+1)(y+2)(3y+2)]^{\frac{1}{2}}}$	$\frac{\{(y+2)(y-6)-2S^2(y-1)(3y+10)\}}{2S[2(2S-1)(2S+1)(y-1)(y+4)(y+2)(3y+2)]^{\frac{1}{2}}}$
$S-1\ S-1;\ 11$	$S\ S-1$	$-\frac{1}{S}\left[\frac{(y+2-2S)}{(3y+2)}\right]^{\frac{1}{2}}$	$\frac{\{S(3y+2)-2(y-6)\}}{4S}\left[\frac{(y+2-2S)}{2(y-1)(y+4)(3y+2)}\right]^{\frac{1}{2}}$
$S-1\ S-2;\ 11$	$S\ S-1$	$-\left[\frac{(2S-3)(y+2S)(y+2-2S)}{(2S-1)(y+2)(3y+2)}\right]^{\frac{1}{2}}$	$\frac{(y+14)}{4}\left[\frac{(2S-3)(y+2S)(y+2-2S)}{2(2S-1)(y-1)(y+4)(y+2)(3y+2)}\right]^{\frac{1}{2}}$
$S\ S-1;\ 10$	$S\ S-1$	$\left[\frac{4S(S+1)}{(y+2)(3y+2)}\right]^{\frac{1}{2}}$	$\frac{\{(y+2)(3y+2)-2S(y+14)\}[(S+1)]^{\frac{1}{2}}}{4[2S(y-1)(y+4)(y+2)(3y+2)]^{\frac{1}{2}}}$
$S-1\ S-1;\ 10$	$S\ S-1$	0	$-\left[\frac{(S-1)(y+2-2S)(3y+2)}{32S(y-1)(y+4)}\right]^{\frac{1}{2}}$
$S\ S-1;\ 01$	$S\ S-1$	$\left[\frac{4(S-1)S}{(y+2)(3y+2)}\right]^{\frac{1}{2}}$	$-\frac{\{(y+2)(3y+2)+2S(y+14)\}[(S-1)]^{\frac{1}{2}}}{4[2S(y-1)(y+4)(y+2)(3y+2)]^{\frac{1}{2}}}$
$S\ S;\ 01$	$S\ S-1$	0	$-\left[\frac{(S+1)(y+2+2S)(3y+2)}{32S(y-1)(y+4)}\right]^{\frac{1}{2}}$

$$\left\langle \begin{matrix}[y11]\ [211] \\ T_1S_1;\ T_2S_2\end{matrix} \middle\| \begin{matrix}[y11] \\ (S-1)S\end{matrix} \right\rangle_\rho = +\left\langle \begin{matrix}[y11]\ [211] \\ S_1T_1;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y11] \\ S(S-1)\end{matrix} \right\rangle_\rho.$$

TABLE A5.1.

S_2T_2	$\left\langle \begin{matrix}[yy0]\ [22] \\ ST;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[yy0] \\ ST\end{matrix} \right\rangle$
00	$\dfrac{\{T(T+1)-S(S+1)\}}{[2y(y+1)(y+3)(y+4)]^{\frac{1}{2}}}$
02	$-\{(y+1)(y+3)+T(T+1)-S(S+1)\}\left[\dfrac{T(T+1)}{2(2T-1)(2T+3)y(y+1)(y+3)(y+4)}\right]^{\frac{1}{2}}$
20	$\{(y+1)(y+3)+S(S+1)-T(T+1)\}\left[\dfrac{S(S+1)}{2(2S-1)(2S+3)y(y+1)(y+3)(y+4)}\right]^{\frac{1}{2}}$

TABLE A5.2.

S_2T_2	$\left\langle \begin{matrix}[yy0]\ [422] \\ ST;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[yy0] \\ ST\end{matrix} \right\rangle$
00	$\dfrac{\{5S(S+1)+5T(T+1)-2y(y+4)\}}{3[6y(y-1)(y+4)(y+5)]^{\frac{1}{2}}}$
02	$\frac{1}{3}\{7T(T+1)+S(S+1)-y(y+4)-9\}\left[\dfrac{5T(T+1)}{6(2T-1)(2T+3)y(y-1)(y+4)(y+5)}\right]^{\frac{1}{2}}$
20	$\frac{1}{3}\{7S(S+1)+T(T+1)-y(y+4)-9\}\left[\dfrac{5S(S+1)}{6(2S-1)(2S+3)y(y-1)(y+4)(y+5)}\right]^{\frac{1}{2}}$

TABLE A5.3.

S_2T_2	$\left\langle \begin{matrix}[y00]\ [422] \\ SS;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y00] \\ SS\end{matrix} \right\rangle$
00	$\dfrac{\{20S(S+1)-3y(y+4)\}}{12[y(y-1)(y+4)(y+5)]^{\frac{1}{2}}}$
02 20	$\dfrac{1}{3}\left[\dfrac{5S(S+1)(2S+3)(2S-1)}{y(y-1)(y+4)(y+5)}\right]^{\frac{1}{2}}$

TABLE A6.1.

S_2T_2	$\left\langle \begin{matrix}[y\ y-1\ 0]\ [22] \\ ST;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y\ y-1\ 0] \\ ST\end{matrix} \right\rangle$
00	$\dfrac{\{T(T+1)-S(S+1)\}}{[2(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}}$
20	$\dfrac{\{(y+1)(y+2)+S(S+1)-T(T+1)\}}{4[2(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}}\left[\dfrac{(2S-1)(2S+3)}{S(S+1)}\right]^{\frac{1}{2}}$
02	$-\dfrac{\{(y+1)(y+2)+T(T+1)-S(S+1)\}}{4[2(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}}\left[\dfrac{(2T-1)(2T+3)}{T(T+1)}\right]^{\frac{1}{2}}$

TABLE A6.2.

S_2T_2	ρ	$\left\langle \begin{matrix}[y\ y-1\ 0]\ [422] \\ ST;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y\ y-1\ 0] \\ ST\end{matrix} \right\rangle^{\frac{1}{2}}$
00	1	$\dfrac{\{(4y^2+12y-1)-10S(S+1)-10T(T+1)\}}{6[2(y-1)(y+4)(3y^2+9y-2)]^{\frac{1}{2}}}$
00	2	$\dfrac{\sqrt{5}\{(2y+3)[y(y+3)-4S(S+1)-4T(T+1)]+(-1)^{y-S-T}(3y^2+9y-2)(S+\frac{1}{2})(T+\frac{1}{2})\}}{3[3(y-1)(y+1)(y-2)(y+2)(y+4)(y+5)(3y^2+9y-2)]^{\frac{1}{2}}}$
02	1	$\dfrac{\{(y+1)(y+2)-S(S+1)-7T(T+1)\}}{12[2(y-1)(y+4)(3y^2+9y-2)]^{\frac{1}{2}}}\left[\dfrac{5(2T-1)(2T+3)}{T(T+1)}\right]^{\frac{1}{2}}$
02	2	$\dfrac{\{(2y+3)[(7y^2+21y+6)-4S(S+1)-28T(T+1)]+(-1)^{y-S-T}(3y^2+9y-2)(2S+1)(2T+1)\}}{12[3(y-1)(y+1)(y-2)(y+2)(y+4)(y+5)(3y^2+9y-2)]^{\frac{1}{2}}}\left[\dfrac{(2T-1)(2T+3)}{T(T+1)}\right]^{\frac{1}{2}}$
20	1	$\dfrac{\{(y+1)(y+2)-T(T+1)-7S(S+1)\}}{12[2(y-1)(y+4)(3y^2+9y-2)]^{\frac{1}{2}}}\left[\dfrac{5(2S-1)(2S+3)}{S(S+1)}\right]^{\frac{1}{2}}$
20	2	$\dfrac{\{(2y+3)[(7y^2+21y+6)-4(TT+1)-28S(S+1)]+(-1)^{y-S-T}(3y^2+9y-2)(2S+1)(2T+1)\}}{12[3(y-1)(y+1)(y-2)(y+2)(y+4)(y+5)(3y^2+9y-2)]^{\frac{1}{2}}}\left[\dfrac{(2S-1)(2S+3)}{S(S+1)}\right]^{\frac{1}{2}}$

TABLE A6.3.

S_2T_2	ST	$\left\langle \begin{matrix}[y11]\ [22] \\ ST;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y11] \\ ST\end{matrix} \right\rangle$
00	$S\ S$	0
20 02	$S\ S$	$\pm\frac{1}{4}\left[\dfrac{(2S-1)(2S+3)(y+2)}{2S(S+1)(y-1)}\right]^{\frac{1}{2}}$
11	$S\ S$	0
00	$S\ S-1$	$\mp\dfrac{S}{[2(y-1)(y+2)]^{\frac{1}{2}}}$
00	$S-1\ S$	
20	$S\ S-1$	$\mp\dfrac{(y+2-2S)}{4}\left[\dfrac{(2S+3)(S+1)}{2S(2S-1)(y-1)(y+2)}\right]^{\frac{1}{2}}$
02	$S-1\ S$	
02	$S\ S-1$	$\pm\dfrac{(y+2+2S)}{4}\left[\dfrac{(2S-3)(S-1)}{2S(2S+1)(y-1)(y+2)}\right]^{\frac{1}{2}}$
20	$S-1\ S$	
11	$S\ S-1$	0
11	$S-1\ S$	

TABLE A6.4.

S_2T_2	ST	ρ	$\left\langle \begin{matrix}[y11]\ [422] \\ ST;\ S_2T_2\end{matrix} \middle\| \begin{matrix}[y11] \\ ST\end{matrix} \right\rangle_\rho$
00	ST	1	$\dfrac{\{(3y+2)(y+2)-10S(S+1)-10T(T+1)\}}{4[3(y-1)(y+4)(y+2)(3y+1)]^{\frac{1}{2}}}$
00	SS	2	$-\dfrac{\{3(y+2)(5y+4)+4(2y-11)S(S+1)\}}{2[6(y-1)(y-2)(y+2)(y+4)(y+5)(3y+1)]^{\frac{1}{2}}}$
00	$S\,S-1$ $S-1\,S$	2	$-\dfrac{\{3(y+2)(5y+4)-4(y+12)S^2\}}{2[6(y-1)(y-2)(y+2)(y+4)(y+5)(3y+1)]^{\frac{1}{2}}}$
02 20	SS	1	$\dfrac{\{(y+2)-4S(S+1)\}}{4}\left[\dfrac{5(2S+3)(2S-1)}{3S(S+1)(y-1)(y+4)(y+2)(3y+1)}\right]^{\frac{1}{2}}$
02 20	SS	2	$\dfrac{\{(y+2)^2(3y-13)-8(2y-11)S(S+1)\}}{4}\times\left[\dfrac{(2S+3)(2S-1)}{30S(S+1)(y-1)(y-2)(y+2)(y+4)(y+5)(3y+1)}\right]^{\frac{1}{2}}$
02 20	$S\,S-1$ $S-1\,S$	1	$-\dfrac{\{y+2+8S^2+6S\}}{4}\left[\dfrac{5(2S-3)(S-1)}{3S(2S+1)(y-1)(y+4)(y+2)(3y+1)}\right]^{\frac{1}{2}}$
02 20	$S\,S-1$ $S-1\,S$	2	$-\dfrac{\{(y+2)^2(3y-13)-6S(3y^2+9y+26)-16S^2(y+12)\}[(2S-3)(S-1)]^{\frac{1}{2}}}{4[30S(2S+1)(y-1)(y-2)(y+2)(y+4)(y+5)(3y+1)]^{\frac{1}{2}}}$
02 20	$S-1\,S$ $S\,S-1$	1	$-\dfrac{\{y+2+8S^2-6S\}}{4}\left[\dfrac{5(2S+3)(S+1)}{3S(2S-1)(y-1)(y+4)(y+2)(3y+1)}\right]^{\frac{1}{2}}$
02 20	$S-1\,S$ $S\,S-1$	2	$-\dfrac{\{(y+2)^2(3y-13)+6S(3y^2+9y+26)-16S^2(y+12)\}[(2S+3)(S+1)]^{\frac{1}{2}}}{4[30S(2S-1)(y-1)(y-2)(y+2)(y+4)(y+5)(3y+1)]^{\frac{1}{2}}}$

TABLE A7.1. $U([yy0][1^3][yy0][1];\ [f^{(12)}][f^{(23)}])$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211]
$[y\,y-1\,0]$	$-\left[\dfrac{y}{2(y+2)}\right]^{\frac{1}{2}}$	$\left[\dfrac{(y+4)}{2(y+2)}\right]^{\frac{1}{2}}$
$[y+1\,y+1\,1]$	$\left[\dfrac{(y+4)}{2(y+2)}\right]^{\frac{1}{2}}$	$\left[\dfrac{y}{2(y+2)}\right]^{\frac{1}{2}}$
Σ_1	n	$-2[y(y+4)]^{\frac{1}{2}}$

TABLE A7.2. $U([y\,y-1\,0][1^3][y\,y-1\,0][1];\ [f^{(12)}],\ [f^{(23)}]\rho_{1,23})$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211] $\rho=1$	[211] $\rho=2$
$[y-1\,y-1\,0]$	$\left[\dfrac{y+1}{8(y+3)}\right]^{\frac{1}{2}}$	$\dfrac{-(y+1)(2y+13)}{[8(y+1)(y+3)(4y^2+12y-1)]^{\frac{1}{2}}}$	$-\left[\dfrac{3(y-1)(y+2)(y+4)}{(y+3)(4y^2+12y-1)}\right]^{\frac{1}{2}}$
$[y\,y-2\,0]$	$-\left[\dfrac{3(y-1)}{8(y+1)}\right]^{\frac{1}{2}}$	$(2y+5)\left[\dfrac{3(y-1)}{8(y+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\left[\dfrac{(y+2)(y+4)}{(4y^2+12y-1)}\right]^{\frac{1}{2}}$
$[y+1\,y\,1]$	$\left[\dfrac{(y+2)(y+4)}{2(y+1)(y+3)}\right]^{\frac{1}{2}}$	$(2y-1)\left[\dfrac{(y+2)(y+4)}{2(y+1)(y+3)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\left[\dfrac{3(y-1)}{(y+3)(4y^2+12y-1)}\right]^{\frac{1}{2}}$
Σ_1	n	$-[4y^2+12y-1]^{\frac{1}{2}}$	0

TABLE A7.3. $U([yy1][1^3][yy1][1];\ [f^{(12)}],\ [f^{(23)}]\rho_{1,23})$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211] $\rho = 1$	[211] $\rho = 2$
[yy0]	$-\left[\frac{y+2}{8y}\right]^{\frac{1}{2}}$	$\frac{-(2y-7)[(y+2)]^{\frac{1}{2}}}{[8y(4y^2+12y-1)]^{\frac{1}{2}}}$	$-\left[\frac{3(y-1)(y+1)(y+4)}{y(4y^2+12y-1)}\right]^{\frac{1}{2}}$
[y y − 1 1]	$-\left[\frac{(y-1)(y+1)}{2y(y+2)}\right]^{\frac{1}{2}}$	$\frac{(2y+7)[(y-1)(y+1)]^{\frac{1}{2}}}{[2y(y+2)(4y^2+12y-1)]^{\frac{1}{2}}}$	$\left[\frac{3(y+4)}{y(4y^2+12y-1)}\right]^{\frac{1}{2}}$
[y + 1 y + 1 2]	$\left[\frac{3(y+4)}{8(y+2)}\right]^{\frac{1}{2}}$	$\frac{(2y+1)[3(y+4)]^{\frac{1}{2}}}{[8(y+2)(4y^2+12y-1)]^{\frac{1}{2}}}$	$-\left[\frac{(y-1)(y+1)}{4y^2+12y-1}\right]^{\frac{1}{2}}$
Σ_1	n	$-[4y^2+12y-1]^{\frac{1}{2}}$	0

TABLE A7.4. $U([y][1^3][y][1];\ [f^{(12)}][f^{(23)}])$

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211]
[y − 1 00]	$\left[\frac{y}{4(y+3)}\right]^{\frac{1}{2}}$	$-\left[\frac{3(y+4)}{4(y+3)}\right]^{\frac{1}{2}}$
[y + 1 11]	$\left[\frac{3(y+4)}{4(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{y}{4(y+3)}\right]^{\frac{1}{2}}$
Σ_1	n	$-[3y(y+4)]^{\frac{1}{2}}$

TABLE A7.5. $U([y11][1^3][y11][1];\ [f^{(12)}],\ [f^{(23)}]\rho_{1,23})$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211] $\rho = 1$	[211] $\rho = 2$
[y10]	$-\left[\frac{(y+2)}{4(y+1)}\right]^{\frac{1}{2}}$	$-\frac{(y-6)}{[4(y+1)(3y+2)]^{\frac{1}{2}}}$	$\left[\frac{2(y-1)(y+4)}{(y+1)(3y+2)}\right]^{\frac{1}{2}}$
[y + 1 22]	$\left[\frac{(y+4)}{2(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+2)(y+4)}{2(y+3)(3y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(y-1)(y+2)}{(y+3)(3y+2)}\right]^{\frac{1}{2}}$
[y − 1 11]	$\left[\frac{(y-1)(y+2)}{4(y+1)(y+3)}\right]^{\frac{1}{2}}$	$-\frac{(3y+10)[y-1]^{\frac{1}{2}}}{[4(y+1)(y+3)(3y+2)]^{\frac{1}{2}}}$	$\left[\frac{8(y+4)}{(y+1)(y+3)(3y+2)}\right]^{\frac{1}{2}}$
Σ_1	n	$-[(y+2)(3y+2)]^{\frac{1}{2}}$	0

TABLE A7.6. $U([y\,y-1\,y-1][1^3][y\,y-1\,y-1][1];\ [f^{(12)}],\ [f^{(23)}]\rho_{1,23})$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211] $\rho = 1$	[211] $\rho = 2$
[y − 1 y − 1 y − 1]	$\left[\frac{(y+2)}{12(y+3)}\right]^{\frac{1}{2}}$	$-\frac{(y+14)}{[12(y+3)(3y+2)]^{\frac{1}{2}}}$	$\left[\frac{8(y-1)(y+4)}{3(y+3)(3y+2)}\right]^{\frac{1}{2}}$
[y + 1 y y]	$\left[\frac{(y+2)(y+4)}{4y(y+3)}\right]^{\frac{1}{2}}$	$\frac{(3y-2)[y+4]^{\frac{1}{2}}}{[4y(y+3)(3y+2)]^{\frac{1}{2}}}$	$\left[\frac{8(y-1)}{y(y+3)(3y+2)}\right]^{\frac{1}{2}}$
[y y − 1 y − 2]	$-\left[\frac{2(y-1)}{3y}\right]^{\frac{1}{2}}$	$\left[\frac{2(y-1)(y+2)}{3y(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+2)(y+4)}{3y(3y+2)}\right]^{\frac{1}{2}}$
Σ_1	n	$-[(y+2)(3y+2)]^{\frac{1}{2}}$	0

TABLE A7.7. $U([y10][1^3][y10][1];\ [f^{(12)}][f^{(23)}]\rho_{1,23})$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211] $\rho = 1$	[211] $\rho = 2$
$[y00]$	$-\left[\frac{y+1}{12y}\right]^{\frac{1}{2}}$	$\frac{-(y-11)}{[12y(3y+7)]^{\frac{1}{2}}}$	$-\left[\frac{8(y-1)(y+4)}{3y(3y+7)}\right]^{\frac{1}{2}}$
$[y-1\ 10]$	$\left[\frac{(y-1)(y+1)}{4y(y+3)}\right]^{\frac{1}{2}}$	$\frac{-3(y+11)[y-1]^{\frac{1}{2}}}{[4y(y+3)(3y+7)]^{\frac{1}{2}}}$	$-\left[\frac{8(y+4)}{y(y+3)(3y+7)}\right]^{\frac{1}{2}}$
$[y+1\ 21]$	$\left[\frac{2(y+4)}{3(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{2(y+1)(y+4)}{3(y+3)(3y+7)}\right]^{\frac{1}{2}}$	$-\left[\frac{(y-1)(y+1)}{3(y+3)(3y+7)}\right]^{\frac{1}{2}}$
Σ_1	n	$-[(y+1)(3y+7)]^{\frac{1}{2}}$	0

TABLE A8.1. $U([yy0][1^2][yy0][1^2];\ [f^{(12)}][f^{(23)}])$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211]	[22]
$[y+1\ y+1\ 0]$	$\left[\frac{(y+3)(y+4)}{6(y+1)(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{y(y+3)}{2(y+1)(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{y}{3(y+2)}\right]^{\frac{1}{2}}$
$[y-1\ y-1\ 0]$	$\left[\frac{y(y+1)}{6(y+2)(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+1)(y+4)}{2(y+2)(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+4)}{3(y+2)}\right]^{\frac{1}{2}}$
$[y+1\ y1]$	$-\left[\frac{2y(y+4)}{3(y+1)(y+3)}\right]^{\frac{1}{2}}$	$-\left[\frac{2}{(y+1)(y+3)}\right]^{\frac{1}{2}}$	$\frac{1}{\sqrt{3}}$
Σ_2	n_+	$\frac{1}{4}(n+2)[3y(y+4)]^{\frac{1}{2}}$	$\frac{1}{2}[2y(y+1)(y+3)(y+4)]^{\frac{1}{2}}$

TABLE A8.2. $U([yy0][2^3][yy0][2];\ [f^{(12)}][f^{(23)}])$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211]	[422]
$[y\ y-2\ 0]$	$\left[\frac{3y(y-1)}{10(y+1)(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{(y-1)(y+4)}{2(y+1)(y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+4)(y+5)}{5(y+1)(y+2)}\right]^{\frac{1}{2}}$
$[y+1\ y1]$	$-\left[\frac{2y(y+4)}{5(y+1)(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{6}{(y+1)(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{3(y-1)(y+5)}{5(y+1)(y+3)}\right]^{\frac{1}{2}}$
$[y+2\ y+2\ 2]$	$\left[\frac{3(y+4)(y+5)}{10(y+2)(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{y(y+5)}{2(y+2)(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{y(y-1)}{5(y+2)(y+3)}\right]^{\frac{1}{2}}$
Σ_2	n_-	$-\frac{1}{4}(n-2)[15y(y+4)]^{\frac{1}{2}}$	$\frac{1}{2}[6y(y-1)(y+4)(y+5)]^{\frac{1}{2}}$

TABLE A8.3. $U([y00][1^2][y00][1^2];\ [f^{(12)}][f^{(23)}])$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211]
$[y+1\ 10]$	$\left[\frac{y+4}{2(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{y}{2(y+2)}\right]^{\frac{1}{2}}$
$[y\ 11]$	$-\left[\frac{y}{2(y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{(y+4)}{2(y+2)}\right]^{\frac{1}{2}}$
Σ_2[a]	n_+	$\frac{3}{8}(n-y)[y(y+4)]^{\frac{1}{2}}$

[a] With $[y00] \to [yyy]$, for $[f^{(23)}] = [211]$; $\Sigma_2 \to \frac{3}{8}(n+y+4)[y(y+4)]^{\frac{1}{2}}$.

TABLE A8.4. $U([y00][2^3][y00][2];\ [f^{(12)}][f^{(23)}])$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211]	[422]
$[y-2\ 00]$	$\left[\frac{y(y-1)}{10(y+2)(y+3)}\right]^{\frac{1}{2}}$	$-\left[\frac{(y-1)(y+4)}{2(y+2)(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{2(y+4)(y+5)}{5(y+2)(y+3)}\right]^{\frac{1}{2}}$
$[y11]$	$\left[\frac{3y}{10(y+2)}\right]^{\frac{1}{2}}$	$\frac{-(y+8)}{[6(y+2)(y+4)]^{\frac{1}{2}}}$	$-\left[\frac{8(y-1)(y+5)}{15(y+2)(y+4)}\right]^{\frac{1}{2}}$
$[y+2\ 22]$	$\left[\frac{3(y+5)}{5(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{y(y+5)}{3(y+3)(y+4)}\right]^{\frac{1}{2}}$	$\left[\frac{y(y-1)}{15(y+3)(y+4)}\right]^{\frac{1}{2}}$
Σ_2	n_-	$-_6(3n+y-4)[5y(y+4)]$	$[y(y-1)(y+4)(y+5)]^{\frac{1}{2}}$

TABLE A8.5. $U([y\ y-1\ 0][1^2][y\ y-1\ 0][1^2];\ [f^{(12)}],\ [f^{(23)}]\rho_{1,23})$.[a]

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[22]	[211] $\rho=1$	[211] $\rho=2$
$[y+1\ y\ 0]$	$\left[\frac{(y+4)}{6y}\right]^{\frac{1}{2}}$	$\left[\frac{(y-1)(y+1)}{3y(y+2)}\right]^{\frac{1}{2}}$	$-\frac{(2y-1)[y+4]^{\frac{1}{2}}}{[2y(4y^2+12y-1)]^{\frac{1}{2}}}$	$\left[\frac{3(y-1)(y+1)}{y(y+2)(4y^2+12y-1)}\right]^{\frac{1}{2}}$
$[y-1\ y-2\ 0]$	$\left[\frac{(y-1)}{6(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+2)(y+4)}{3(y+1)(y+3)}\right]^{\frac{1}{2}}$	$\frac{(2y+7)[y-1]^{\frac{1}{2}}}{[2(y+3)(4y^2+12y-1)]^{\frac{1}{2}}}$	$-\left[\frac{3(y+2)(y+4)}{(y+1)(y+3)(4y^2+12y-1)}\right]^{\frac{1}{2}}$
$[yy1]$	$-\frac{1}{\sqrt{6}}$	$\left[\frac{(y-1)(y+4)}{12(y+1)(y+2)}\right]^{\frac{1}{2}}$	$\frac{-5}{[2(4y^2+12y-1)]^{\frac{1}{2}}}$	$-\frac{(2y+3)[3(y-1)(y+4)]^{\frac{1}{2}}}{2[(y+1)(y+2)(4y^2+12y-1)]^{\frac{1}{2}}}$
$[y+1\ y-1\ 1]$	$-\left[\frac{(y-1)(y+4)}{2y(y+3)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+1)(y+2)}{4y(y+3)}\right]^{\frac{1}{2}}$	$-\left[\frac{3(y-1)(y+4)}{2y(y+3)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{(2y+3)[(y+1)(y+2)]^{\frac{1}{2}}}{2[y(y+3)(4y^2+12y-1)]^{\frac{1}{2}}}$
Σ_2	n_+	$\frac{1}{2}[2(y-1)(y+1)(y+2)(y+4)]^{\frac{1}{2}}$	$\frac{\sqrt{3}\{(y-1)(y+1)(2y+7)+x(4y^2+12y-1)\}}{2[(4y^2+12y-1)]^{\frac{1}{2}}}$	$-\frac{3}{2}\left[\frac{2(y-1)(y+1)(y+2)(y+4)}{(4y^2+12y-1)}\right]^{\frac{1}{2}}$

[a] $U([yy1][1^2][yy1][1^2];\ [f^{(12)}][f^{(23)}]\rho) = (-1)^{\rho+1}U([yy-1\ 0][1^2][y\ y-1\ 0][1^2];\ [f^{(12)*}][f^{(23)}]\rho)$. The Σ_2 values are the same as the above except for [211] $\rho=1$ for which $\Sigma_2 = \{\sqrt{3}[(y+1)(y+2)(2y+3)+x(4y^2+12y-1)]\}/\{2[(4y^2+12y-1)]^{\frac{1}{2}}\}$.

TABLE A8.6. $U([y\,y-1\,0][2^3][y\,y-1\,0][2];\ [f^{(12)}], [f^{(23)}]\rho_{1,23})$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211] $\rho=1$	[211] $\rho=2$	[422] $\rho=1$	[422] $\rho=2$
$[y-1\,y-2\,0]$	$-\left[\frac{y-1}{10(y+3)}\right]^{\frac{1}{2}}$	$\frac{(2y+11)[y-1]^{\frac{1}{2}}}{[6(y+3)(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{(4y-5)[(y+2)(y+4)]^{\frac{1}{2}}}{3[(y+1)(y+3)(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{(3y+22)[y+4]^{\frac{1}{2}}}{3[5(y+3)(3y^2+9y-2)]^{\frac{1}{2}}}$	$-\left[\frac{2(y-2)(y+2)(y+4)(y+5)}{3(y+1)(y+3)(3y^2+9y-2)}\right]^{\frac{1}{2}}$
$[yy1]$	$\frac{1}{\sqrt{10}}$	$\frac{-3\sqrt{3}}{[2(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{-2(y+11)[(y-1)(y+2)]^{\frac{1}{2}}}{2[(y+1)(y+4)(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{(3y+22)[y-1]^{\frac{1}{2}}}{2[5(y+4)(3y^2+9y-2)]^{\frac{1}{2}}}$	$-\left[\frac{3(y-1)(y-2)(y+2)(y+5)}{2(y+1)(y+4)(3y^2+9y-2)}\right]^{\frac{1}{2}}$
$[y\,y-3\,0]$	$\left[\frac{(y-1)(y-2)}{5y(y+1)}\right]^{\frac{1}{2}}$	$\frac{-(2y+5)[(y-1)(y-2)]^{\frac{1}{2}}}{[3y(y+1)(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{2}{3}\left[\frac{2(y-2)(y+2)(y+4)}{y(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{-2(3y+7)[(y-2)(y+4)]^{\frac{1}{2}}}{3[10y(y+1)(3y^2+9y-2)]^{\frac{1}{2}}}$	$-\left[\frac{(y+2)(y+4)(y+5)}{3y(3y^2+9y-2)}\right]^{\frac{1}{2}}$
$[y+1\,y-1\,1]$	$-\left[\frac{3(y-1)(y+4)}{10y(y+3)}\right]^{\frac{1}{2}}$	$5\left[\frac{(y-1)(y+4)}{2y(y+3)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{-(2y^2+11y+32)[y+1]^{\frac{1}{2}}}{2[3y(y+2)(y+3)(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{-(9y^2+17y-56)}{2[15y(y+3)(3y^2+9y-2)]^{\frac{1}{2}}}$	$\frac{-(y+4)[(y+1)(y-2)(y+5)]^{\frac{1}{2}}}{[2y(y+2)(y+3)(3y^2+9y-2)]^{\frac{1}{2}}}$
$[y+2\,y+1\,2]$	$\left[\frac{3(y+5)}{10(y+1)}\right]^{\frac{1}{2}}$	$\frac{(2y-1)[y+5]^{\frac{1}{2}}}{[2(y+1)(4y^2+12y-1)]^{\frac{1}{2}}}$	$-\left[\frac{3(y-1)(y+5)}{(y+2)(y+4)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{-(y-1)[3(y-1)(y+5)]^{\frac{1}{2}}}{[5(y+1)(y+4)(3y^2+9y-2)]^{\frac{1}{2}}}$	$-\left[\frac{2(y-1)(y-2)}{(y+2)(y+4)(3y^2+9y-2)}\right]^{\frac{1}{2}}$
Σ_2	n_-	$\frac{-3\sqrt{5}\left\{\begin{matrix}(y-1)(y+3)(2y-1)\\ +x(4y^2+12y-1)\end{matrix}\right\}}{2[3(4y^2+12y-1)]^{\frac{1}{2}}}$	$-\left[\frac{5(y-1)(y+1)(y+2)(y+4)}{2(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\frac{1}{2}[2(y-1)(y+4)(3y^2+9y-2)]^{\frac{1}{2}}$	0

TABLE A8.7. $U([yy1][2^3][yy1][2];\ [f^{(12)}], [f^{(23)}]\rho_{1,23})$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211] $\rho=1$	[211] $\rho=2$	[422] $\rho=1$	[422] $\rho=2$
$[y+1\,y+1\,1]$	$-\left[\frac{y+4}{10y}\right]^{\frac{1}{2}}$	$-\frac{(2y-5)[y+4]^{\frac{1}{2}}}{[6y(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{-(4y+17)[(y-1)(y+1)]^{\frac{1}{2}}}{3[y(y+2)(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{(3y-13)[y-1]^{\frac{1}{2}}}{[45y(3y^2+9y-2)]^{\frac{1}{2}}}$	$-\left[\frac{2(y-1)(y+1)(y-2)(y+5)}{3y(y+2)(3y^2+9y-2)}\right]^{\frac{1}{2}}$
$[y\,y-1\,0]$	$\frac{1}{\sqrt{10}}$	$\frac{-3\sqrt{3}}{[2(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{(2y-5)[(y+1)(y+4)]^{\frac{1}{2}}}{2[(y-1)(y+2)(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{(3y-13)[y+4]^{\frac{1}{2}}}{2[5(y-1)(3y^2+9y-2)]^{\frac{1}{2}}}$	$-\left[\frac{3(y+1)(y-2)(y+4)(y+5)}{2(y-1)(y+2)(3y^2+9y-2)}\right]^{\frac{1}{2}}$
$[y+2\,y+2\,3]$	$\left[\frac{(y+4)(y+5)}{5(y+2)(y+3)}\right]^{\frac{1}{2}}$	$\frac{(2y+1)[(y+4)(y+5)]^{\frac{1}{2}}}{[3(y+2)(y+3)(4y^2+12y-1)]^{\frac{1}{2}}}$	$-\frac{2}{3}\left[\frac{2(y-1)(y+1)(y+5)}{(y+3)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{-(3y+2)[2(y-1)(y+5)]^{\frac{1}{2}}}{3[5(y+2)(y+3)(3y^2+9y-2)]^{\frac{1}{2}}}$	$-\left[\frac{(y-1)(y+1)(y-2)}{3(y+3)(3y^2+9y-2)}\right]^{\frac{1}{2}}$
$[y+1\,y\,2]$	$-\left[\frac{3(y-1)(y+4)}{10y(y+3)}\right]^{\frac{1}{2}}$	$5\left[\frac{(y-1)(y+4)}{2y(y+3)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{(2y^2+y+17)[y+2]^{\frac{1}{2}}}{2[3y(y+1)(y+3)(4y^2+12y-1)]^{\frac{1}{2}}}$	$\frac{-(9y^2+37y-26)}{2[15y(y+3)(3y^2+9y-2)]^{\frac{1}{2}}}$	$\frac{-(y-1)[(y-2)(y+2)(y+5)}{[2y(y+1)(y+3)(3y^2+9y-2)]^{\frac{1}{2}}}$
$[y\,y-2\,1]$	$\left[\frac{3(y-2)}{10(y+2)}\right]^{\frac{1}{2}}$	$\frac{-(2y+7)[y-2]^{\frac{1}{2}}}{[2(y+2)(4y^2+12y-1)]^{\frac{1}{2}}}$	$-\left[\frac{3(y-2)(y+4)}{(y-1)(y+1)(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$\frac{-(y+4)[3(y-2)(y+4)]^{\frac{1}{2}}}{[5(y-1)(y+2)(3y^2+9y-2)]^{\frac{1}{2}}}$	$\left[\frac{2(y+4)(y+5)}{(y-1)(y+1)(3y^2+9y-2)}\right]^{\frac{1}{2}}$
Σ_2	n_-	$\frac{-\sqrt{15}\left\{\begin{matrix}(y-1)(2y^2+7y+2)\\ +x(4y^2+12y-1)\end{matrix}\right\}}{2[(4y^2+12y-1)]^{\frac{1}{2}}}$	$-\left[\frac{5(y-1)(y+1)(y+2)(y+4)}{2(4y^2+12y-1)}\right]^{\frac{1}{2}}$	$-\frac{1}{2}[2(y-1)(y+4)(3y^2+9y-2)]^{\frac{1}{2}}$	0

TABLE A8.8. $U([y11][1^2][y11][1^2];\ [f^{(12)}],\ [f^{(23)}]\rho_{1,23})$.[a]

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211] $\rho=1$	[211] $\rho=2$	[22]
[y00]	$-\frac{1}{3}\left[\frac{y+2}{2y}\right]^{\frac{1}{2}}$	$\frac{(y-6)}{[6y(3y+2)]^{\frac{1}{2}}}$	$-\left[\frac{4(y-1)(y+4)}{3y(3y+2)}\right]^{\frac{1}{2}}$	$\frac{2}{3}\left[\frac{(y-1)}{y}\right]^{\frac{1}{2}}$
[y − 1 10]	$-\left[\frac{(y-1)(y+2)}{6y(y+3)}\right]^{\frac{1}{2}}$	$\frac{-(y+6)[y-1]^{\frac{1}{2}}}{[2y(y+3)(3y+2)]^{\frac{1}{2}}}$	$\frac{-(y-2)[y+4]^{\frac{1}{2}}}{[y(y+3)(3y+2)]^{\frac{1}{2}}}$	$\frac{-(y+2)}{[3y(y+3)]^{\frac{1}{2}}}$
[y + 1 21]	$\frac{2}{3}\left[\frac{(y+2)(y+4)}{(y+1)(y+3)}\right]^{\frac{1}{2}}$	$\frac{-2y[y+4]^{\frac{1}{2}}}{[3(y+1)(y+3)(3y+2)]^{\frac{1}{2}}}$	$\frac{-(y-2)[y-1]^{\frac{1}{2}}}{[6(y+1)(y+3)(3y+2)]^{\frac{1}{2}}}$	$\frac{1}{3}\left[\frac{(y-1)(y+4)}{2(y+1)(y+3)}\right]^{\frac{1}{2}}$
[y22]	$-\left[\frac{(y-1)}{3(y+1)}\right]^{\frac{1}{2}}$	$-\left[\frac{(y-1)(y+2)}{(y+1)(3y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+2)(y+4)}{2(y+1)(3y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{(y+2)}{6(y+1)}\right]^{\frac{1}{2}}$
Σ_2	n_+	$\frac{\{2(y+4)+x(3y+2)\}}{2}\left[\frac{3(y+2)}{(3y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{6(y-1)(y+2)(y+4)}{(3y+2)}\right]^{\frac{1}{2}}$	$[2(y-1)(y+2)]^{\frac{1}{2}}$

[a] $U([yy-1\ y-1][1^2][y\ y-1\ y-1][1^2];\ [f^{(12)}],[f^{(23)}]\rho)=(-1)^{\rho+1}\,U([y11][1^2][y11][1^2];\ [f^{(12)*}],[f^{23}]\rho)$. The Σ_2 values are the same as the above except for [211] $\rho=1$ for which $\Sigma_2=\frac{1}{2}[3(y+2)(y-1)+x(3y+2)][3(y+2)/(3y+2)]^{\frac{1}{2}}$.

TABLE A8.9. $U([y11][2^3][y11][2];\ [f^{(12)}],\ [f^{(23}]\rho_{1,23})$.

$[f^{(12)}]$ \ $[f^{(23)}]$	[0]	[211] $\rho=1$	[211] $\rho=2$	[422] $\rho=1$	[422] $y=2$
[y − 1 10]	$-\left[\frac{(y-1)(y+2)}{10y(y+3)}\right]^{\frac{1}{2}}$	$\frac{(y+10)[y-1]^{\frac{1}{2}}}{[6y(y+3)(3y+2)]^{\frac{1}{2}}}$	$\frac{(y-4)[y+4]^{\frac{1}{2}}}{[3y(y+3)(3y+2)]^{\frac{1}{2}}}$	$\frac{-(2y-11)[2(y+4)]^{\frac{1}{2}}}{[15y(y+3)(3y+1)]^{\frac{1}{2}}}$	$\left[\frac{5(y-2)(y+4)(y+5)}{3y(y+3)(3y+1)}\right]^{\frac{1}{2}}$
[y − 2 11]	$\left[\frac{(y-1)(y-2)}{10y(y+3)}\right]^{\frac{1}{2}}$	$\frac{-(3y+10)[(y-1)(y-2)]^{\frac{1}{2}}}{[6y(y+3)(y+2)(3y^2+2)]^{\frac{1}{2}}}$	$4\left[\frac{(y-2)(y+4)}{3y(y+3)(y+2)(3y+2)}\right]^{\frac{1}{2}}$	$\frac{-(3y+11)[2(y-2)(y+4)]^{\frac{1}{2}}}{[15y(y+3)(y+2)(3y+1)]^{\frac{1}{2}}}$	$2\left[\frac{5(y+4)(y+5)}{3y(y+3)(y+2)(3y+1)}\right]^{\frac{1}{2}}$
[y22]	$\left[\frac{(y-1)}{5(y+1)}\right]^{\frac{1}{2}}$	$\frac{-(y+6)[y-1]^{\frac{1}{2}}}{[3(y+1)(y+2)(3y+2)]^{\frac{1}{2}}}$	$\frac{(y^2+4y+20)}{[6(y+1)(y+4)(y+2)(3y+2)]^{\frac{1}{2}}}$	$\frac{(4y^2+19y+2)}{[15(y+1)(y+2)(y+4)(3y+1)]^{\frac{1}{2}}}$	$y\left[\frac{5(y-2)(y+5)}{6(y+1)(y+2)(y+4)(3y+1)}\right]^{\frac{1}{2}}$
[y + 1 21]	$-\left[\frac{4(y+2)(y+4)}{15(y+1)(y+3)}\right]^{\frac{1}{2}}$	$\frac{-2(y-4)[y+4]^{\frac{1}{2}}}{3[(y+1)(y+3)(3y+2)]^{\frac{1}{2}}}$	$\frac{(5y+22)[y-1]^{\frac{1}{2}}}{3[2(y+1)(y+3)(3y+2)]^{\frac{1}{2}}}$	$\frac{(2y-11)[y-1]^{\frac{1}{2}}}{3[5(y+1)(y+3)(3y+1)]^{\frac{1}{2}}}$	$-\frac{1}{3}\left[\frac{5(y-1)(y-2)(y+5)}{2(y+1)(y+3)(3y+1)}\right]^{\frac{1}{2}}$
[y + 2 33]	$\left[\frac{(y+5)}{3(y+3)}\right]^{\frac{1}{2}}$	$\frac{1}{3}\left[\frac{5(y+2)(y+5)}{(y+3)(3y+2)}\right]^{\frac{1}{2}}$	$\frac{1}{3}\left[\frac{10(y-1)(y+2)(y+5)}{(y+3)(y+4)(3y+2)}\right]^{\frac{1}{2}}$	$-\frac{1}{3}\left[\frac{(y-1)(y+2)(y+5)}{(y+3)(y+4)(3y+1)}\right]^{\frac{1}{2}}$	$-\frac{1}{3}\left[\frac{2(y-1)(y-2)(y+2)}{(y+3)(y+4)(3y+1)}\right]^{\frac{1}{2}}$
Σ_2[a]	n_-	$-\frac{\{(y-1)(y+2)+x(3y+2)\}}{2}\left[\frac{15(y+2)}{(3y+2)}\right]^{\frac{1}{2}}$	$\left[\frac{10(y-1)(y+2)(y+4)}{3(3y+2)}\right]^{\frac{1}{2}}$	$-\left[\frac{(y-1)(y+2)(y+4)(3y+1)}{3}\right]^{\frac{1}{2}}$	0

[a] If $[y11]\rightarrow[y\ y-1\ y-1]$, the Σ_2 values are the same as above except for [211] $\rho=1$ for which $\Sigma_2=-\frac{1}{2}\{2(y-1)y+x(3y+2)\}[15(y+2)/(3y+2)]^{\frac{1}{2}}$.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

On the Renormalization of the Susceptibility of a Fermi Liquid

DANIEL J. AMIT*
Department of Theoretical Physics, The Hebrew University, Jerusalem, Israel

(Received 10 February 1969)

It is shown that the susceptibility of a normal Fermi liquid can be renormalized without using Ward identities for the derivatives of the mass operator with respect to the magnetic field. The procedure is completely analogous to the renormalization of the compressibility. The result which expresses the susceptibility in terms of Landau parameters is correct only to lowest order in temperature. The behavior of higher-order terms in temperature is discussed.

1. INTRODUCTION

It has been shown by Nozières and Luttinger[1] and others[2,3] that one can derive the results of the phenomenological Landau theory[4] from a microscopic theory. For this purpose one has to identify the following in the microscopic theory: (1) the quasiparticle energy,[1] and (2) the Landau parameters.[1,5] The first is identified as the real part of the pole of the single-particle Green's function. The second is taken to be the limits of the vertex function multiplied by the square of the renormalization constant.

When these identifications have been made, one obtains the equation for the propagation of zero sound[5] in the same form as in the phenomenological theory. Furthermore, using Ward identities, one obtains the equations for the effective mass of a quasiparticle and the compressibility.[1,3] If one defines the Fermi momentum as the momentum at which the quasiparticle energy vanishes, then one can also show[6] that the usual relation between particle number and the volume of the Fermi sphere holds. This result was extended by Dzyaloshinski[7] to show that the magnetic moment of the normal Fermi liquid is proportional to the difference of the volumes of the Fermi sphere for quasiparticles with spin up and the one for quasiparticles with spin down.

In this work we show that the susceptibility of the normal Fermi liquid can be renormalized in a microscopic theory without using Ward identities for the derivatives of the mass operator with respect to the magnetic field. This can be done provided the interactions are spin-independent. In that case the number of particles with each spin projection is conserved and the Ward identity connecting the derivatives of the mass operator with respect to frequency to the vertex function holds, regardless of whether we use the symmetric or antisymmetric part of the vertex function. See, e.g., Eq. (12) below. This is sufficient to make the renormalization of the susceptibility identical to that of the compressibility.

The result is as in Ref. 4:

$$\chi = \frac{m^*}{m}\chi^0(1 - A_0^a) = \frac{m^*}{m}\chi^0(1 + F_0^a)^{-1}, \qquad (1)$$

where m is the mass of the fermion, m^* the effective mass, χ^0 the Pauli susceptibility of a free gas, and A_0^a the angular average of the antisymmetric part of the forward-scattering amplitude of two quasiparticles on the Fermi surface. (We use here the notation of Ref. 8 for the Landau parameters. In the notation of Ref. 4, we have $F_0^a = \bar{\psi}_0$.)

After proving this result, we show it to be correct only to lowest order in temperature. However, the only approximation made is in isolating the coherent part of the particle–hole propagator. The error made is of relative order T^2 and so is the correction term in the susceptibility.

2. BASIC FORMULAS

We treat a normal system of fermions using the temperature-dependent Green's-function formalism.[1,8,9] The system is described by a single-particle Green's function $G(1 - 1')$, where $1 = (r_1, t_1)$ and $t_1 \in (0, -i\beta)$. The Hamiltonian is assumed to be spin-independent and to contain only two-body forces. Thus, the only spin-dependent effects are due

* Present address: Department of Physics, Brandeis University, Waltham, Mass.

[1] P. Nozières and J. M. Luttinger, Phys. Rev. **127**, 1423, 1431 (1962).

[2] L. P. Pitayevski, Zh. Eksp. Teor. Fiz. **37**, 1794 (1959) [Sov. Phys.—JETP **10**, 1267 (1960)].

[3] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, N.J., 1963).

[4] L. D. Landau, Zh. Eksp. Teor. Fiz. **30**, 1058 (1956); **32**, 59 (1957) [Sov. Phys.—JETP **3**, 920 (1956); **5**, 101 (1957)].

[5] L. D. Landau, Zh. Eksp. Teor. Fiz. **35**, 97 (1958) [Sov. Phys.—JETP **8**, 70 (1959)].

[6] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).

[7] I. E. Dzyaloshinski, Zh. Eksp. Teor. Fiz. **46**, 1722 (1964) [Sov. Phys.—JETP **19**, 1163 (1964)].

[8] D. J. Amit, J. W. Kane, and H. Wagner, Phys. Rev. Letters **19**, 425 (1967); Phys. Rev. **175**, 313 (1968).

[9] D. J. Amit, in *Mathematical Methods in Solid State and Superfluid Theory*, R. C. Clark and G. H. Derrick, Eds. (Oliver and Boyd, Edinburgh, 1969).

to exchange. The assumption of spin independence allows us to separate every two-particle (four-point) function into its direct and exchange parts, i.e.,

$$G_{\alpha\beta\gamma\delta}(11', 22') = \tfrac{1}{2}[G_1\delta_{\alpha\gamma}\delta_{\beta\delta} + G_2\boldsymbol{\sigma}_{\alpha\gamma}\cdot\boldsymbol{\sigma}_{\beta\delta}], \quad (2)$$

where α, β, γ, δ are spin indices and $\boldsymbol{\sigma}$ are Pauli matrices. The two-particle Green's function is conventionally defined as

$$G_{\alpha\beta\gamma\delta}(11', 22') \equiv -\langle T[\psi_\alpha(1)\psi_\beta(1')\psi^+_\delta(2')\psi^+_\gamma(2)]\rangle. \quad (3)$$

The magnetic moment of the system in a weak magnetic field $\mathbf{H}$ is given by[10]

$$\begin{aligned}\mathbf{M} &= -\mu_0 \lim_{2\to 1^+}\Big\{ i\int d^4 2' \langle T[\psi_\alpha(1)\psi^+_\delta(2')\psi_\beta(2')\psi^+_\gamma(2)]\rangle\boldsymbol{\sigma}_{\gamma\alpha} \\ &\quad\cdot(\boldsymbol{\sigma}_{\delta\beta}\cdot\mathbf{H}) \\ &= -\mu_0^2 i\Big[\int d^4 2' G_{\alpha\beta\gamma\delta}(11', 22')\big|_{1'=2'^+}\Big]_{2=1^+}\boldsymbol{\sigma}_{\gamma\alpha}(\boldsymbol{\sigma}_{\delta\beta}\cdot\mathbf{H}),\end{aligned} \quad (4)$$

where

$$\int d^4 1 = \int d^3 r_1 \int_0^{-i\beta} dt_1, \quad 1^+ = (\mathbf{r}_1, t_1 + 0),$$

and μ_0 is the Bohr magneton.

Inserting in (4) the decomposition (2) of G, we find

$$\mathbf{M} = -2\mu_0^2 i\Big[\int d^4 2' G_2(11', 22')\big|_{1'=2'^+}\Big]_{2=1^+}\cdot\mathbf{H}, \quad (5)$$

which is the expected result that $\mathbf{M}$ is in the direction of $\mathbf{H}$. The susceptibility is, therefore,

$$\chi = -2\mu_0^2\Big[i\int d^4 2' G_2(11', 22')\big|_{1'=2'^+}\Big]_{2=1^+}. \quad (6)$$

Writing G_2 in momentum space in terms of particle–hole variables, we define

$$\begin{aligned}&G_2(11', 22') \\ &\quad= (-i\beta\Omega)^{-3}\sum_{p,q,q'} G_2(p; q, q') \\ &\qquad\times \exp\{i[p(1-2') + q(1-2) + q'(1'-2')]\}\end{aligned} \quad (7)$$

where $p\cdot 1 = \mathbf{p}\cdot\mathbf{r}_1 - p_0 t_1$ [we use

$$(\beta\Omega)^{-1}\sum_q = \frac{1}{\beta}\sum_{q_0}\int\frac{d^3 q}{(2\pi)^3}, \quad \text{where} \quad \sum_{q_0}$$

is the sum over the discrete imaginary frequencies], Ω is the volume of the system, and $\beta = (k_B T)^{-1}$. Inserting in (6), we get

$$\chi = \mu_0^2\frac{2i}{(\beta\Omega)^2}\sum_{q,q'} G_2^k(q, q')e^{(q_0'0^+ - q_0 0^+)}. \quad (8)$$

G_2^k is the "k limit"[5] of $G_2(p; q, q')$. [We henceforth drop the explicit $\exp(q_0'0^+ - q_0 0^+)$, as it will not be needed.]

The two-particle Green's function is related to the vertex part Γ via[1,9]

$$\begin{aligned}G_{\alpha\beta\gamma\delta}(p; q, q') &= R_q(q' - q)(-i\beta\Omega)\delta_{p,0}\delta_{\alpha\gamma}\delta_{\beta\delta} \\ &\quad - R_q(p)(-i\beta\Omega)\cdot\delta_{qq'}\delta_{\alpha\delta}\delta_{\beta\gamma} \\ &\quad + iR_q(p)\Gamma_{\alpha\beta\gamma\delta}(p; q, q')R_{q'}(p).\end{aligned} \quad (9)$$

R is simply the product of two Green's functions, namely

$$R_q(p) = G(q)G(q + p).$$

Using (2) and (9), we find

$$\begin{aligned}\chi &= -2\mu_0^2(\beta\Omega)^{-1}\sum_q R_q^k\Big[1 + (\beta\Omega)^{-1}\sum_{q'}\Gamma_2^k(q, q')R_{q'}^k\Big] \\ &= -2\mu_0^2 S_2^k,\end{aligned} \quad (10)$$

where we defined S_i^k by

$$S_i^k = (\beta\Omega)^{-1}\sum_q R_q^k\Big[1 + (\beta\Omega)^{-1}\sum_{q'}\Gamma_i^k(q, q')R_q^k\Big]. \quad (11)$$

S_i^k is the same as S^{00k}, the static correlation function of Ref. 1 after a spin decomposition. Finally, we note that the compressibility K is given by[1]

$$K = -(N\rho)^{-1}S_1^k,$$

where $N = \rho\Omega$ is the number of particles.

3. WARD IDENTITY

The Ward identity relating the frequency derivative of the mass operator M to the vertex part, Eq. (4.18) of Ref. 1, can be derived from the conservation of the number of particles in the system,[11] together with the assumption of two-body forces. Since it is the number of particles of each spin species that is conserved, we obtain[8]

$$\frac{\partial M(q)}{\partial q_0} = -(\beta\Omega)^{-1}\sum_{q'}\Gamma_i^\omega(q, q')R_{q'}^\omega, \quad i = 1, 2. \quad (12)$$

In particular, setting q on the Fermi surface we obtain

$$\begin{aligned}a_f^{-1} &= 1 - \frac{\partial M(k_F\omega)}{\partial\omega}\bigg|_{\omega=0} \\ &= 1 + (\beta\Omega)^{-1}\sum_{q'}\Gamma_i^\omega(\mathbf{n}, q')R_{q'}^\omega, \quad i = 1, 2.\end{aligned} \quad (13)$$

In other words, the renormalization constant is given by the same expression, whether we use Γ_1 or Γ_2.

Finally, we make use of the identity

$$\sum_q R_q^\omega\Big[1 - \frac{\partial M(q)}{\partial q_0}\Big] = 0 \quad (14)$$

[10] A. A. Abrikosov and L. P. Gorkov, Zh. Eksp. Teor. Fiz. 39, 480 (1960) [Sov. Phys.—JETP 12, 337 (1961)].

[11] J. R. Schrieffer, *Theory of Superconductivity* (W. A. Benjamin, Inc., New York, 1964).

[see Eq. (5.16) of Ref. 1]. Together with Eq. (12) this leads to

$$\sum_q R_q^\omega \left[1 + (\beta\Omega)^{-1} \sum_{q'} \Gamma_i^\omega(q, q') R_{q'}^\omega\right] = 0. \quad (15)$$

4. LOW-MOMENTUM TRANSFER BEHAVIOR

We turn now to the low-momentum transfer behavior of the quantities involved. We have[1]

$$R_q^k = R_q^\omega - \beta a_f \tilde{\delta}_q [1 + O(\beta^{-2}\mu^{-2})]. \quad (16)$$

R_q^ω is the "ω limit"[5] of R, a_f is the renormalization constant, and

$$\tilde{\delta}_q = (1/v_F)\delta(|q| - k_F)\delta_{q_0,0}, \quad (17)$$

where $v_F = k_F/m^*$ is the quasiparticle velocity. This relation can be proved to all orders in perturbation theory at $T = 0$,[12] and at finite T it can be checked in low-order diagrams or in an RPA calculation.

Furthermore, using the renormalized Bethe–Salpeter equation at low-momentum transfer, which is called Landau's equation, one finds,[8,9] for $i = 1, 2$, that

$$\Gamma_i^\omega(q, q') - \Gamma_i^k(q, q') = a_f^2 N^*(0) \int \frac{d\mathbf{n}''}{4\pi} \Gamma_i^k(q, \mathbf{n}'') \Gamma_i^\omega(\mathbf{n}'', q'), \quad (18)$$

where the appearance of the unit vector $\mathbf{n}''$ in Γ indicates $\mathbf{q}'' = \mathbf{n}'' k_F$, $q_0'' = 0$, i.e., the four-momentum is set on the Fermi surface, $N^*(0) = m^* k_F/2\pi^2$. The integral in Eq. (18) is over the unit sphere. Equation (18) has again corrections of relative order $(\beta\mu)^{-2}$, since Eq. (16) is used in deriving it.

From Eq. (18), we have

$$(\beta\Omega)^{-1} \sum_{q'} \{\Gamma_i^\omega(q, q') R_{q'}^\omega - \Gamma_i^k(q, q') R_{q'}^k + \Gamma_i^k(q, q')(R_{q'}^k - R_{q'}^\omega)\} = a_f^2 N^*(0) \int \frac{d\mathbf{n}''}{4\pi} \Gamma_i^k(q, \mathbf{n}'') \left[(\beta\Omega)^{-1} \sum_{q'} \Gamma_i^\omega(\mathbf{n}'', q') R_{q'}^\omega\right].$$

In the last term of the left-hand side, we insert Eq. (16), and the term in brackets on the right-hand side is expressed in terms of the renormalization constant by using Eq. (13). Thus, we arrive at

$$\frac{1}{\beta\Omega} \sum_{q'} [\Gamma_i^\omega(q, q') R_{q'}^\omega - \Gamma_i^k(q, q') R_{q'}^k] = a_f N^*(0) \int \frac{d\mathbf{n}'}{4\pi} \Gamma_i^k(q, \mathbf{n}'), \quad (19)$$

and this equation, again, holds for both $i = 1$ and 2.

[12] J. M. Luttinger, Phys. Rev. **121**, 942 (1961).

Setting (19) on the Fermi surface and using (13) gives

$$(\beta\Omega)^{-1} \sum_{q'} \Gamma_i^k(\mathbf{n}, q') R_{q'}^k = (a_f^{-1} - 1) - a_f N^*(0) \int \frac{d\mathbf{n}'}{4\pi} \Gamma_i^k(\mathbf{n}, \mathbf{n}'). \quad (20)$$

5. THE RENORMALIZATION OF S_i^k

Using (16) and (19), we can write S_i^k as

$$S_i^k = (\beta\Omega)^{-1} \sum_q (R_q^\omega - \beta a_f^2 \tilde{\delta}_q) \times \left[1 + (\beta\Omega)^{-1} \sum_{q'} \Gamma_i^\omega(q, q') R_{q'}^\omega\right] - (\beta\Omega)^{-1} a_f N^*(0) \sum_q \int \frac{d\mathbf{n}'}{4\pi} R_q^k \Gamma_i^k(q, \mathbf{n}'). \quad (21)$$

Next we use (15) and (13) to rewrite it as

$$S_i^k = -a_f N^*(0) \left[1 + \int \frac{d\mathbf{n}'}{4\pi} (\beta\Omega)^{-1} \sum_q \Gamma_i^k(\mathbf{n}', q) R_q^k\right], \quad (22)$$

where in the last term we used the fact that $\Gamma^k(q, q')$ is symmetric in q and q'. Finally, we insert (20) in (22) to find

$$S_i^k = -N^*(0) + [a_f N^*(0)]^2 \int \frac{dn}{4\pi} \Gamma_i^k(\mathbf{n}, \mathbf{n}'). \quad (23)$$

At $T = 0$, the second term reduces to $N^*(0)A_0^s$ when $i = 1$, where A_0^s is the angular average of the symmetric part of the scattering amplitude, and to $N^*(0)A_0^a$ when $i = 2$; thus,

$$S_i^k(T = 0) = -N^*(0)[1 - A_0^{s,a}] = -N^*(0)[1 + F_0^{s,a}]^{-1}. \quad (24)$$

6. THE COMPRESSIBILITY AND SUSCEPTIBILITY

From (24) and the expression for K and χ, we obtain Landau's results, i.e.,

$$K = (N\rho)^{-1} N^*(0)(1 - A_0^s), \quad (25)$$

$$\chi = 2\mu_0^2 N^*(0)(1 - A_0^a) \quad (26)$$

at $T = 0$.

In Eq. (22), Γ_i^k is temperature-dependent, but it is easy to convince oneself that the equation gives only the $T = 0$ term correctly. In order to see this it is enough to look at the system of noninteracting fermions. In this case

$$S_i^{k(0)} = \int \frac{q^2\, dq}{2\pi^2} f'(\epsilon_q^0),$$

where f' is the derivative of the Fermi distribution function and $\epsilon_q^0 = (q^2 - k_F^2)/2m$. At $T = 0$,

$$S_i^{k(0)} = -N(0) = -mk_F/2\pi^2.$$

If in Eq. (24) we set $A_0^{s,a} = 0$, $m^* = m$, which corresponds to the case of the noninteracting system, we obtain the $T = 0$ result.

The difference, clearly, comes from the approximation made in Eq. (16). This equation introduces errors of relative order T^2 in Eq. (19) and finally in Eq. (21). As is suggested by the comparison with the noninteracting system, Eq. (16) becomes exact at $T = 0$.[6] This is the form in which it was used in Ref. 8.

The correction to the zero-temperature susceptibility has been calculated through the paramagnon approximation.[13] It was found to behave like T^2, and by using the approximate expression for the free energy the coefficient was explicitly calculated.

ACKNOWLEDGMENT

Many invaluable discussions with Dr. Herbert Wagner are gratefully acknowledged.

[13] M. T. Beal-Monod, Shang-Keng Ma, and D. R. Fredkin, Phys. Rev. Letters **20**, 929 (1968).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

New Formulation of Stochastic Theory and Quantum Mechanics

L. DE LA PEÑA-AUERBACH*
Instituto de Física, Universidad Nacional de México, México, D.F.

(Received 31 January 1969)

The theory of stochastic motion is formulated from a new point of view. It is shown that the fundamental equations of the theory reduce to Schrödinger's equation for specific values of certain parameters. A generalized Fokker–Planck–Kolmogorov equation is obtained; with other values of the parameters, certain approximations reduce this to the Smoluchowski equation for Brownian movement. In particular, the potential function in the Schrödinger equation differs in the two cases. The usual uncertainty relations appear in a natural way in the theory, but in a broader context. A single theory thus covers both similarities and differences between quantum-mechanical and Brownian motion. Furthermore, possibilities for broadening nonrelativistic quantum mechanics are brought out and, as an example, the possible corrections due to non-Markoffian terms are briefly studied.

I. INTRODUCTION

In this paper we are concerned once more with the possibility of giving a stochastic foundation to quantum mechanics. In this sense it continues a series of earlier papers,[1–3] although the problem is here approached from a new point of view and in a much more general form.

The basic idea is developed as follows: In the first place we construct a new formulation of stochastic theory (Sec. II) using two guiding principles, namely, that the theory must be an extension of Newtonian mechanics and that the velocities and the forces must transform according to certain rules with respect to time-inversion. These rules are indeed sufficient to establish the two fundamental differential equations of the theory, which, in a particular but interesting case, reduce to the set first given by Nelson.[4] Once the theory is constructed, we show without further physical assumptions that Schrödinger's equation is a first integral of our fundamental stochastic equations (Sec. III). In fact, the equation we obtain is more general than Schrödinger's, which is obtained by fixing certain parameters of the theory. In this form we see that it is possible to reinterpret quantum-mechanics as a stochastic process. Then we turn back to our basic set of equations and show that their first integrals may be written alternatively as a continuity and an energy-conservation equation (Sec. IV). The first of these may be cast into the form of a generalized Fokker–Planck–Kolmogorov equation of the type discussed by Pawula[5] and gives, as we show, the Smoluchowski equation[6] for Brownian motion if

* Technical consultant, Comisión Nacional de Energía Nuclear, México.

[1] L. de la Peña-Auerbach, Phys. Letters **24A**, 603 (1967).

[2] L. de la Peña-Auerbach, E. Braun, and L. García-Colín, J. Math. Phys. **9**, 668 (1968).

[3] L. de la Peña-Auerbach and L. García-Colín, J. Math. Phys. **9**, 916, 922 (1968); Rev. Mex. Fís. **16**, 221 (1967).

[4] E. Nelson, Phys. Rev. **150**, 1079 (1966). See also by the same author: *Dynamical Theories of Brownian Motion* (Princeton University Press, Princeton, N.J., 1967).

[5] R. F. Pawula, IEEE Trans. Inform. Theory **13**, 33 (1967); Phys. Rev. **162**, 186 (1967).

[6] S. Chandrasekhar, Rev. Mod. Phys. **15**, 1 (1943). Reprinted in *Selected Papers of Noise and Stochastic Processes*, N. Wax, Ed. (Dover Publications, Inc., New York, 1954).

If in Eq. (24) we set $A_0^{s,a} = 0$, $m^* = m$, which corresponds to the case of the noninteracting system, we obtain the $T = 0$ result.

The difference, clearly, comes from the approximation made in Eq. (16). This equation introduces errors of relative order T^2 in Eq. (19) and finally in Eq. (21). As is suggested by the comparison with the noninteracting system, Eq. (16) becomes exact at $T = 0$.[6] This is the form in which it was used in Ref. 8.

The correction to the zero-temperature susceptibility has been calculated through the paramagnon approximation.[13] It was found to behave like T^2, and by using the approximate expression for the free energy the coefficient was explicitly calculated.

ACKNOWLEDGMENT

Many invaluable discussions with Dr. Herbert Wagner are gratefully acknowledged.

[13] M. T. Beal-Monod, Shang-Keng Ma, and D. R. Fredkin, Phys. Rev. Letters **20**, 929 (1968).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

New Formulation of Stochastic Theory and Quantum Mechanics

L. DE LA PEÑA-AUERBACH*
Instituto de Física, Universidad Nacional de México, México, D.F.

(Received 31 January 1969)

The theory of stochastic motion is formulated from a new point of view. It is shown that the fundamental equations of the theory reduce to Schrödinger's equation for specific values of certain parameters. A generalized Fokker–Planck–Kolmogorov equation is obtained; with other values of the parameters, certain approximations reduce this to the Smoluchowski equation for Brownian movement. In particular, the potential function in the Schrödinger equation differs in the two cases. The usual uncertainty relations appear in a natural way in the theory, but in a broader context. A single theory thus covers both similarities and differences between quantum-mechanical and Brownian motion. Furthermore, possibilities for broadening nonrelativistic quantum mechanics are brought out and, as an example, the possible corrections due to non-Markoffian terms are briefly studied.

I. INTRODUCTION

In this paper we are concerned once more with the possibility of giving a stochastic foundation to quantum mechanics. In this sense it continues a series of earlier papers,[1–3] although the problem is here approached from a new point of view and in a much more general form.

The basic idea is developed as follows: In the first place we construct a new formulation of stochastic theory (Sec. II) using two guiding principles, namely, that the theory must be an extension of Newtonian mechanics and that the velocities and the forces must transform according to certain rules with respect to time-inversion. These rules are indeed sufficient to establish the two fundamental differential equations of the theory, which, in a particular but interesting case, reduce to the set first given by Nelson.[4] Once the theory is constructed, we show without further physical assumptions that Schrödinger's equation is a first integral of our fundamental stochastic equations (Sec. III). In fact, the equation we obtain is more general than Schrödinger's, which is obtained by fixing certain parameters of the theory. In this form we see that it is possible to reinterpret quantum-mechanics as a stochastic process. Then we turn back to our basic set of equations and show that their first integrals may be written alternatively as a continuity and an energy-conservation equation (Sec. IV). The first of these may be cast into the form of a generalized Fokker–Planck–Kolmogorov equation of the type discussed by Pawula[5] and gives, as we show, the Smoluchowski equation[6] for Brownian motion if

* Technical consultant, Comisión Nacional de Energía Nuclear, México.

[1] L. de la Peña-Auerbach, Phys. Letters **24A**, 603 (1967).

[2] L. de la Peña-Auerbach, E. Braun, and L. García-Colín, J. Math. Phys. **9**, 668 (1968).

[3] L. de la Peña-Auerbach and L. García-Colín, J. Math. Phys. **9**, 916, 922 (1968); Rev. Mex. Fís. **16**, 221 (1967).

[4] E. Nelson, Phys. Rev. **150**, 1079 (1966). See also by the same author: *Dynamical Theories of Brownian Motion* (Princeton University Press, Princeton, N.J., 1967).

[5] R. F. Pawula, IEEE Trans. Inform. Theory **13**, 33 (1967); Phys. Rev. **162**, 186 (1967).

[6] S. Chandrasekhar, Rev. Mod. Phys. **15**, 1 (1943). Reprinted in *Selected Papers of Noise and Stochastic Processes*, N. Wax, Ed. (Dover Publications, Inc., New York, 1954).

some approximations, equivalent to the transition to the static limit, are made. In this latter case, a parameter λ which characterizes the interaction of the particle with its surroundings takes a value different from that needed in the quantum-mechanical case. This interaction parameter appears in an unusual energy term in our generalized Schrödinger equation; hence, the difference in the values it takes are of fundamental importance: if it is unity, the classical quantum-mechanical case is obtained, while a value different from unity gives rise to the equations of Brownian motion and adds a new term to Schrödinger's equation. This means that, although in our theory there is an interaction of the particle with its surroundings, postulated from the beginning, this interaction remains hidden in the quantum-mechanical case but gives rise to a dissipative term in the Brownian case. In this way the stochastic theory here presented allows us to state explicitly the common aspects of quantum mechanics and Brownian motion, making possible at the same time to state the great differences between these two different physical situations.

In deriving Schrödinger's equation from the general theory we truncate *a priori* a Taylor-series development to second order, which is equivalent to considering that the interaction of the particle with its surroundings is Markoffian. To see more clearly the possible consequences of this last hypothesis, we return to the question in Sec. V, in which it is shown that the higher-order terms previously disregarded give rise to a perturbing potential. In particular, it is shown that the fourth-order term in the Taylor development gives, if it is not zero and satisfies certain simplifying assumptions, a correction to the energy levels of a stationary system which has the same form as the dominant radiative corrections in quantum-electrodynamics responsible for the Lamb shift in the hydrogenlike atom, i.e., $\delta E \sim \langle \nabla^2 V \rangle$. This calculation is straightforward but only qualitative, the final result being expressed in terms of an at present unknown parameter. In this form, we cannot reach at present any final answer to the question of the legitimacy or illegitimacy of our truncating the Taylor expansion to second order, but we hope that an extension of the present work which is in course may be of value in getting more definitive results about this point.

Some results of this paper were obtained previously along different lines of thought,[1-4] but it seems to us that the method here set forth is more direct and that the physical content of the theory is clearer, the formulation being more general and enlightening. For a discussion of some related topics, as for example the introduction of the usual operators into the theory, which are barely touched upon in this paper, the interested reader may refer to the literature.[2,3]

II. THE FUNDAMENTAL EQUATIONS OF THE STOCHASTIC THEORY

The scope of this section is to derive from first principles the equations of motion of a classical particle subject simultaneously to the action of an external and a stochastic force, this last being generated by the interaction of the particle with the medium through which it moves. We assume that the velocity $\mathbf{c}$ of the particle may be written as the sum of a systematic or current velocity $\mathbf{v}$ and a stochastic component $\mathbf{u}$[4]:

$$\mathbf{c} = \mathbf{v} + \mathbf{u}. \tag{1}$$

Let us introduce the time-reversal operation which consists in the transformation $\mathbf{x} \to \mathbf{x}$, $t \to -t$; in other words, in the change of the direction of the time axis. We shall denote it by $\hat{T}$ and write for short $\hat{T}f = \tilde{f}$, f being any quantity on which $\hat{T}$ acts. The effect of $\hat{T}$ on f is to replace t by $-t$ everywhere in f. In classical as well as in quantum mechanics, the transformation properties under $\hat{T}$ of the kinematic and dynamic variables are usually inferred from their definition; for example, the velocity of a classical particle, being the limit of $\Delta\mathbf{x}/\Delta t$ as $\Delta t \to 0$ is supposed to reverse its sign under $\hat{T}$. We here also impose upon the velocities $\mathbf{v}$ and $\mathbf{u}$ a well-defined behavior under time reversal and, in particular, we assume that they transform under $\hat{T}$ as follows:

$$\tilde{\mathbf{v}} = -\mathbf{v},$$
$$\tilde{\mathbf{u}} = +\mathbf{u}. \tag{2}$$

In the limit when the stochastic force goes to zero (in what follows called the Newtonian limit) we want to recover Newtonian mechanics; this establishes the first of Eqs. (2). On the other hand, the transformation property of $\mathbf{u}$ implies that in the Newtonian limit $\mathbf{u} = 0$ necessarily, because in this limit we must have $\tilde{\mathbf{c}} = -\mathbf{c}$. Equations (2) imply that the velocities $\mathbf{v}$ and $\mathbf{u}$ are essentially different variables, $\mathbf{v}$ being the velocity in Newtonian mechanics but $\mathbf{u}$ having no classical analog. We have from (1) and (2) that

$$\tilde{\mathbf{c}} = -\mathbf{v} + \mathbf{u} \tag{3}$$

and so

$$\mathbf{v} = \tfrac{1}{2}(\mathbf{c} - \tilde{\mathbf{c}}),$$
$$\mathbf{u} = \tfrac{1}{2}(\mathbf{c} + \tilde{\mathbf{c}}). \tag{4}$$

In classical mechanics, the velocity $\mathbf{v}$ and the position coordinate $\mathbf{x}$ of a particle are linearly related

through the total time-derivative operator:

$$\mathbf{v} = (d/dt)\mathbf{x}.$$

In order to get a similar relationship in our more general scheme, it is necessary to investigate which operator, if any, may be used in place of d/dt to relate $\mathbf{x}$ (now a stochastic process) with $\mathbf{c} = \mathbf{v} + \mathbf{u}$. Clearly, a relation of the above type will have meaning only in the mean, due to the stochastic nature of the motion which we are assuming. To investigate this question, let us assume on physical grounds that there exists a distribution of the changes in the space coordinate $\delta\mathbf{x} = \mathbf{x}(t + \Delta t) - \mathbf{x}(t)$ which occurs in a small time interval Δt, this distribution being such that its moments in $\delta\mathbf{x}$ divided by Δt all remain finite in the limit $\Delta t \to 0$. In this paper we shall adhere to the following convention: when we take the average of a quantity over the probability density of $\delta\mathbf{x}(\Delta t)$, we shall write this average as $E\{\ \}$ and call it for short the mean or the mean value; on the other hand, if the average is taken over an ensemble of equivalent particles to be introduced later on, we shall call it the average or the average value and write $\langle\ \rangle_{\text{av}}$. The mean, in this restricted sense, is thus the conditional expectation in the interval Δt.[4] Now let us introduce any sufficiently smooth function of $\mathbf{x}$ and t, say $f(\mathbf{x}, t)$, and suppose that it admits a development in a Taylor series about the point $\mathbf{x}, t$; let Δt be a small positive time interval. Then we can write, letting x_i be the components of $\mathbf{x}$,

$$\begin{aligned}\frac{1}{\Delta t}&[f(\mathbf{x}(t+\Delta t), t+\Delta t) - f(\mathbf{x}(t), t)] \\ &\approx \Big[\frac{\partial}{\partial t} + \frac{1}{\Delta t}\sum_i [x_i(t+\Delta t) - x_i(t)]\partial_i \\ &\quad + \frac{1}{2\Delta t}\sum_{i,j}[x_i(t+\Delta t) - x_i(t)] \\ &\quad \times [x_j(t+\Delta t) - x_j(t)]\partial_i\partial_j + \cdots\Big] f(\mathbf{x}(t), t).\end{aligned}$$

Taking the mean of the above expression and passing to the limit $\Delta t \to 0$, we obtain

$$\begin{aligned}\mathfrak{D}f(\mathbf{x}, t) &\equiv \lim_{\Delta t\to 0}\frac{1}{\Delta t}E\{f(\mathbf{x}(t+\Delta t), t+\Delta t) - f(\mathbf{x}(t), t)\} \\ &= \Big[\frac{\partial}{\partial t} + \sum_i c_i\partial_i + \sum_{i,j} D_{ij}\partial_i\partial_j + \cdots\Big] f(\mathbf{x}, t).\end{aligned} \tag{5}$$

Here $c_i, 2D_{ij}, \cdots$ stand for the limits of the first-second-, $\cdots$ order moments of the distribution divided by Δt, and we are identifying c_i with the components of the previously introduced velocity $\mathbf{c}$. For a more detailed mathematical discussion of topics related to ours, the reader is referred to Refs. 4, 6, 7 and references cited therein. In what follows we assume for simplicity that the matrix whose elements are D_{ij} as defined in Eq. (5), is diagonal. Hence we write the above result in the form:

$$\mathfrak{D}f = \frac{\partial f}{\partial t} + \mathbf{c}\cdot\nabla f + D\nabla^2 f + \cdots. \tag{6}$$

Clearly, in the Newtonian limit when D and all higher-order coefficients vanish, $\mathfrak{D}f$ reduces to the usual total time-derivative of f. Also from (6) we have that

$$(\hat{T}\mathfrak{D})f \equiv \tilde{\mathfrak{D}}f = -\frac{\partial f}{\partial t} + \tilde{\mathbf{c}}\cdot\nabla f + \tilde{D}\nabla^2 f + \cdots. \tag{7}$$

If we call $\mathfrak{D}$ the (mean) forward derivative operator, then $\tilde{\mathfrak{D}}$ represents the negative of the (mean) backward derivative operator; for in the Newtonian limit $\tilde{\mathfrak{D}}f$ goes to minus the total time derivative, as follows from (2) and (7). According to (6) and (7), these operators are

$$\begin{aligned}\mathfrak{D} &= \frac{\partial}{\partial t} + \mathbf{c}\cdot\nabla + D\nabla^2 + \cdots, \\ \tilde{\mathfrak{D}} &= -\frac{\partial}{\partial t} + \tilde{\mathbf{c}}\cdot\nabla + \tilde{D}\nabla^2 + \cdots.\end{aligned} \tag{8}$$

Applying (8) to x_i, one gets

$$\begin{aligned}\mathfrak{D}x_i &= c_i, \\ \tilde{\mathfrak{D}}x_i &= \tilde{c}_i.\end{aligned} \tag{9}$$

This result shows that the operators $\mathfrak{D}$ and $\tilde{\mathfrak{D}}$ may in fact be considered as the sought-for generalization of the total time-derivative in classical mechanics, in the sense that with their help we can construct the velocities from the position coordinates. Now using (4) we immediately get

$$\begin{aligned}\mathbf{v} &= \tfrac{1}{2}(\mathfrak{D} - \tilde{\mathfrak{D}})\mathbf{x} = \mathfrak{D}_c\mathbf{x}, \\ \mathbf{u} &= \tfrac{1}{2}(\mathfrak{D} + \tilde{\mathfrak{D}})\mathbf{x} = \mathfrak{D}_s\mathbf{x},\end{aligned} \tag{10}$$

where we have introduced the systematic (or current) derivative operator

$$\mathfrak{D}_c \equiv \tfrac{1}{2}(\mathfrak{D} - \tilde{\mathfrak{D}}) \tag{11a}$$

and the stochastic derivative operator

$$\mathfrak{D}_s \equiv \tfrac{1}{2}(\mathfrak{D} + \tilde{\mathfrak{D}}). \tag{11b}$$

With the help of (4) and (8), Eqs. (11) become

$$\begin{aligned}\mathfrak{D}_c &= \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla - D_-\nabla^2 + \cdots, \\ \mathfrak{D}_s &= \mathbf{u}\cdot\nabla + D_+\nabla^2 + \cdots,\end{aligned} \tag{12}$$

[7] Ming Chen Wang and G. E. Uhlenbeck, Rev. Mod. Phys. 17, 323 (1945). Reprinted in the same book as Ref. 6.

where

$$D_+ = \tfrac{1}{2}(\tilde{D} + D),$$
$$D_- = \tfrac{1}{2}(\tilde{D} - D). \tag{13}$$

Note that in the Newtonian limit, $\mathfrak{D}_s$ acting on any function of $\mathbf{x}$ and t gives zero, which we simply write as $\mathfrak{D}_s = 0$; on the other side, in the same limit $\mathfrak{D}_c$ goes into $\partial/\partial t + \mathbf{v}\cdot\nabla = d/dt$.

Since we want to construct a dynamical theory, we must consider forces in the scheme, which we shall always write per unit mass (p.u.m.) for simplicity. In classical mechanics there is a direct relation between forces and acceleration which we want to extend into the theory. With this aim, we introduce the quantity

$$\mathbf{a} = \mathfrak{D}\mathbf{c}, \tag{14}$$

i.e., the forward derivative of the velocity $\mathbf{c}$; with the aid of (1) and (11) we can rewrite (14) in the form

$$\mathbf{a} = \mathfrak{D}_c\mathbf{v} + \mathfrak{D}_s\mathbf{u} + \mathfrak{D}_c\mathbf{u} + \mathfrak{D}_s\mathbf{v}. \tag{15}$$

In the Newtonian limit, (15) reduces to

$$\mathbf{a} = \mathfrak{D}_c\mathbf{v} = d\mathbf{v}/dt,$$

i.e., the acceleration of the particle, which, according to Newton's second law, is equal to the total force acting on the particle. This suggests that we can give to Eq. (15) a dynamical content if we put $\mathbf{a} = \mathbf{f}$, $\mathbf{f}$ being the (mean) total force (p.u.m.) acting on the particle. Let us consider at this stage only $\hat{T}$-invariant forces, e.g., forces which do not depend on the velocities; then we may assume that $\mathbf{a}$ is also invariant under $\hat{T}$. However, $\mathbf{a}$ as defined in (14) and (15) is not $\hat{T}$-invariant. In fact, since

$$\mathfrak{D}_c = \tfrac{1}{2}(\mathfrak{D} - \tilde{\mathfrak{D}}) = -\tilde{\mathfrak{D}}_c,$$
$$\mathfrak{D}_s = \tfrac{1}{2}(\mathfrak{D} + \tilde{\mathfrak{D}}) = \tilde{\mathfrak{D}}_s,$$

it follows that

$$\tilde{\mathbf{a}} = \mathfrak{D}_c\mathbf{v} + \mathfrak{D}_s\mathbf{u} - \mathfrak{D}_c\mathbf{u} - \mathfrak{D}_s\mathbf{v}. \tag{16}$$

Therefore, if we want $\mathbf{a}$ to be $\hat{T}$-invariant, i.e., $\mathbf{a} = \tilde{\mathbf{a}}$, then a comparison of Eqs. (15) and (16) leads us to the following postulates:

$$\mathfrak{D}_c\mathbf{v} + \mathfrak{D}_s\mathbf{u} = \mathbf{a}, \tag{17a}$$
$$\mathfrak{D}_c\mathbf{u} + \mathfrak{D}_s\mathbf{v} = 0. \tag{17b}$$

Let us now introduce our dynamical postulate: *the total force* (p.u.m.) *acting on the particle is equal to the total acceleration given by Eq.* (17a), i.e.,

$$\mathbf{f} = \mathbf{a}. \tag{18}$$

This postulate guarantees that the system of Eqs. (17) and (18) represents a generalization of Newtonian mechanics, Eqs. (18) and (17a) being the form that the second law takes in the presence of stochastic forces. Equation (17b) is trivially satisfied in the Newtonian limit (when $\mathbf{u}$ and $\mathfrak{D}_s$ are both zero).

For brevity, let us write

$$\mathbf{a} = \mathbf{a}_c + \mathbf{a}_s, \tag{19}$$

where

$$\mathbf{a}_c = \mathfrak{D}_c\mathbf{v} = \mathfrak{D}_c^2\mathbf{x} = \tilde{\mathbf{a}}_c,$$
$$\mathbf{a}_s = \mathfrak{D}_s\mathbf{u} = \mathfrak{D}_s^2\mathbf{x} = \tilde{\mathbf{a}}_s, \tag{20}$$

the second pair of equalities following from (10) and the last one from (2) and (11).

Thus, $\mathbf{a}_c$ is the acceleration associated with the systematic rate of change of the current velocity, whereas $\mathbf{a}_s$ is the acceleration associated with the mean stochastic rate of change of the stochastic velocity. Also, from (17b) we see that the systematic changes of $\mathbf{u}$ are always compensated by the changes impressed by the stochastic motion on $\mathbf{v}$. In this sense, this equation is a kind of action–reaction law.

Explicitly the $\hat{T}$-invariant form of $\mathbf{a}$ reads

$$\mathbf{a} = \tfrac{1}{2}(\mathfrak{D}\mathbf{c} + \tilde{\mathfrak{D}}\tilde{\mathbf{c}}) = \tfrac{1}{2}(\mathfrak{D}^2 + \tilde{\mathfrak{D}}^2)\mathbf{x}. \tag{21}$$

Also,

$$\mathbf{a}_c = \tfrac{1}{4}(\mathfrak{D} - \tilde{\mathfrak{D}})^2\mathbf{x},$$
$$\mathbf{a}_s = \tfrac{1}{4}(\mathfrak{D} + \tilde{\mathfrak{D}})^2\mathbf{x}, \tag{22}$$

and finally, from (17b), we get

$$(\mathfrak{D}_s\mathfrak{D}_c + \mathfrak{D}_c\mathfrak{D}_s)\mathbf{x} = \tfrac{1}{2}(\mathfrak{D}^2 - \tilde{\mathfrak{D}}^2)\mathbf{x} = 0.$$

Now we introduce a last postulate into the theory in order to express the basic equations in terms of the applied external force (p.u.m.) $\mathbf{f}_0$. In general, we may expect the external force to be the fundamental cause of the changes of the systematic motion, although as we have seen the stochastic force may also contribute to them. This means that we may consider the total force $\mathbf{f}_0$ as a superposition of the external force and a component of stochastic origin. Since, on the other hand, the mean total force is given by a linear combination of $\mathbf{a}_c$ and $\mathbf{a}_s$, we may consider that the four quantities $\mathbf{a}_c$, $\mathbf{a}_s$, $\mathbf{f}$, and $\mathbf{f}_0$ are linearly related. Hence, we write

$$\mathbf{f}_0 = \lambda_1\mathbf{a}_c + \lambda_2\mathbf{a}_s.$$

This equation together with $\mathbf{f} = \mathbf{a}_c + \mathbf{a}_s$ allows us to write $\mathbf{f}$ as a linear combination of $\mathbf{f}_0$ and, say, $\mathbf{a}_s$, according to the preceding discussion. From space- and time-translation invariance we conclude that λ_1 and λ_2 must be constants. Furthermore, we require that in the Newtonian limit, i.e., when $\mathbf{a}_s \to 0$, we have $\mathbf{f}_0 = \mathbf{a}_c$, and thus $\lambda_1 = 1$. Finally, writing $-\lambda$ instead of λ_2, we arrive at the following result:

$$\mathbf{f}_0 = \mathbf{a}_c - \lambda\mathbf{a}_s. \tag{23}$$

Equation (23) must be considered as a postulate. In it, λ is left as a parameter of the theory (later on we shall find its value for some cases of interest). Combining (18), (19), and (23), we get that

$$\mathbf{f} = \mathbf{f}_0 + (1 + \lambda)\mathbf{a}_s, \tag{24}$$

where $\mathbf{f}$ is given by (17a). In other words, we have as our fundamental equations the following system:

$$\mathbf{f}_0 = \mathfrak{D}_c\mathbf{v} - \lambda\mathfrak{D}_s\mathbf{u},$$
$$\mathfrak{D}_c\mathbf{u} + \mathfrak{D}_s\mathbf{v} = 0, \tag{25}$$

which, when written out explicitly with the help of Eqs. (12), takes the form

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v} - D_-\nabla^2\mathbf{v} - \lambda(\mathbf{u}\cdot\nabla)\mathbf{v} - \lambda D_+\nabla^2\mathbf{u} + \cdots = \mathbf{f}_0,$$
$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{v} + D_+\nabla^2\mathbf{v} - D_-\nabla^2\mathbf{u} + \cdots = 0. \tag{26}$$

Equations (26), which are a generalization of the system given in earlier papers[2,3] and also of that proposed by Nelson,[4] describe the motion of a particle subject simultaneously to the action of a $\hat{T}$-invariant external force $\mathbf{f}_0$ and a stochastic force generated by the interaction of the particle with its surroundings, under the assumptions that the velocity may be written as the sum $\mathbf{v} + \mathbf{u}$ of a systematic and a stochastic component, each transforming under $\hat{T}$ according to Eq. (2), and that the external force $\mathbf{f}_0$ is related to the total force $\mathbf{f}$ as in Eq. (24) with constant λ.

Since the two velocities $\mathbf{v}$ and $\mathbf{u}$ satisfy a system of coupled equations, they are not independent, the stochastic and systematic motions influencing one another in a complex way. Due to this fact, we may expect that the motion of a particle satisfying Eqs. (26) differs fundamentally from the corresponding Newtonian case. Clearly, in the Newtonian limit when $D_+ = D_- = 0$, etc., the second equation in (26) has the trivial solution $\mathbf{u} = 0$ and then the first one of these equations reduces to Newton's second law $d\mathbf{v}/dt = \mathbf{f}_0$.

Actually the system (26) is more general than needed for our later purposes. Thus in what follows we reduce ourselves to a more particular situation. We shall, in fact, assume first that the coefficients D_+, D_-, etc., depend only on time; secondly, that the velocities $\mathbf{c}$ and $\tilde{\mathbf{c}}$ and in consequence $\mathbf{v}$ and $\mathbf{u}$ are irrotational; and, finally, that the external force may be obtained from a potential V. With these assumptions, we can write Eqs. (26) in the form

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla[\tfrac{1}{2}\mathbf{v}^2 - D_-\nabla\cdot\mathbf{v} - \tfrac{1}{2}\lambda\mathbf{u}^2 - \lambda D_+\nabla\cdot\mathbf{u}] + \cdots = -\nabla V,$$
$$\frac{\partial \mathbf{u}}{\partial t} + \nabla[\mathbf{v}\cdot\mathbf{u} + D_+\nabla\cdot\mathbf{v} - D_-\nabla\cdot\mathbf{u}] + \cdots = 0. \tag{27}$$

This is the system that we use as our basis throughout the remainder of the paper.

III. THE SCHRÖDINGER EQUATION

We will now attempt to show the physical meaning of Eqs. (27) in more usual terms by deriving a Schrödinger equation from them. An alternative and complementary way of tackling the problem appears in the next section.

Equations (27) are a system of coupled nonlinear differential equations. However, for several important cases a first integral may be written which uncouples and linearizes them; the conditions for this case are given later on. Starting from the postulated irrotational character of $\mathbf{v}$ and $\mathbf{u}$, we may write

$$\mathbf{v} = 2D_0\nabla S, \tag{28a}$$
$$\mathbf{u} = 2D_0\nabla R. \tag{28b}$$

Here $R = R(\mathbf{x}, t)$ and $S = S(\mathbf{x}, t)$ are dimensionless real functions of $\mathbf{x}$ and t and D_0 is a constant which may be specified by writing

$$D_+ = D_0\eta_+,$$
$$D_- = D_0\eta_-, \tag{29}$$

where η_+ and η_- are real dimensionless functions of time. When D_+ does not depend on time, it is clear that we may take $\eta_+ = 1$, i.e., $D_+ = D_0$.

In this and the next sections we restrict ourselves to a special case of Eqs. (27), namely, that which is obtained by putting all the coefficients of the terms of order > 2 in the series (12) equal to zero, i.e., by assuming that, for $\Delta t \to 0$, only the first and second moments become proportional to Δt. This point will be commented on in later sections.

With these restrictions we introduce (28) into (27) and integrate to obtain

$$2D_0\frac{\partial S}{\partial t} = -V + 2D_0^2[\eta_-\nabla^2 S - (\nabla S)^2 + \lambda\eta_+\nabla^2 R + \lambda(\nabla R)^2], \tag{30a}$$
$$2D_0\frac{\partial R}{\partial t} = 2D_0^2[\eta_-\nabla^2 R - 2\nabla R\cdot\nabla S - \eta_+\nabla^2 S], \tag{30b}$$

where the "constants" of integration (which may depend on time) are taken as zero, since they may be

absorbed into R and S. Introduce now a complex function ψ given by[1]

$$\psi = \exp(R + iS). \tag{31}$$

Then we can write, from Eqs. (30) and (31),

$$\begin{aligned} 2iD_0\psi^{-1}\frac{\partial\psi}{\partial t} &= 2D_0\left(i\frac{\partial R}{\partial t} - \frac{\partial S}{\partial t}\right) \\ &= 2D_0^2[-i(\eta_+ - i\eta_-)\nabla^2 S + (\nabla S)^2 - 2i\nabla R\cdot\nabla S \\ &\quad - (\lambda\eta_+ - i\eta_-)\nabla^2 R - \lambda(\nabla R)^2] + V. \end{aligned}$$

From (31) it follows that

$$\psi^{-1}\nabla^2\psi = \nabla^2 R + (\nabla R)^2 - (\nabla S)^2 + i[\nabla^2 S + 2\nabla R\cdot\nabla S],$$

which may be used to eliminate, say, $(\nabla S)^2$ from the previous result. We obtain

$$\begin{aligned} 2iD_0\frac{\partial\psi}{\partial t} &= -2D_0^2\nabla^2\psi + V\psi \\ &\quad - 2D_0^2(\eta_+ - 1 - i\eta_-)\psi\nabla^2\ln\psi \\ &\quad - 2D_0^2(\lambda - 1)[(\nabla R)^2 + \eta_+\nabla^2 R]\psi, \end{aligned}$$

where $\nabla^2\ln\psi = \nabla^2 R + i\nabla^2 S$. We can now make use of (31) and its complex conjugate (c.c.) to write the derivatives of R in terms of ψ and ψ^* as follows:

$$\begin{aligned} (\nabla R)^2 + \eta_+\nabla^2 R &= \tfrac{1}{4}(\psi^{-1}\nabla\psi + \psi^{*-1}\nabla\psi^*)^2 \\ &\quad + \tfrac{1}{2}\eta_+\nabla\cdot(\psi^{-1}\nabla\psi + \psi^{*-1}\nabla\psi^*) \\ &= (2D_0^2)^{-1}(\tfrac{1}{2}\mathbf{u}^2 + D_+\nabla\cdot\mathbf{u}), \end{aligned}$$

where $\mathbf{u}$ is to be taken as depending on ψ and ψ^*. The result is

$$2iD_0\frac{\partial\psi}{\partial t} = -2D_0^2\nabla^2\psi + (V + V_C + V_U)\psi, \tag{32}$$

with

$$\begin{aligned} V_C &= -2D_0^2(\eta_+ - 1 - i\eta_-)\nabla^2\ln\psi, \\ V_U &= -(\lambda - 1)(\tfrac{1}{2}\mathbf{u}^2 + D_+\nabla\cdot\mathbf{u}). \end{aligned} \tag{33}$$

Equation (32) and its complex conjugate are a first integral of the fundamental system of stochastic equations (27) expressed in terms of the function ψ and coincide in fact with Schrödinger's equation and its c.c. for a potential (p.u.m.) $V_T = V + V_C + V_U$. This equation and its c.c. are coupled through V_U and are nonlinear due to both V_C and V_U. Thus, to get a linear theory, we must require that $V_C = V_U = 0$, which, at the same time, uncouples Schrödinger's equation from its complex conjugate. From (29) and (33) we see that the condition $V_C = 0$ implies that $\eta_+ = 1$ and $\eta_- = 0$, and hence that $D_+ = D_0 =$ const and $D_- = 0$; also, the condition $V_U = 0$ implies $\lambda = 1$. With these values of D_+, D_-, and λ, Eq. (32) reduces to Schrödinger's equation in its usual form:

$$2iD_0\frac{\partial\psi}{\partial t} = -2D_0^2\nabla^2\psi + V\psi,$$

where V is the potential associated with the external force $\mathbf{f}_0$.

It may be useful to state explicitly what we are implying from the standpoint of the present theory when we write Schrödinger's equation in its usual form. We have just seen that in this case, we need $D_+ = D_0 = \text{const}$ (and moreover $= \hbar/2m$), $D_- = 0$, i.e., $D = \tilde{D}$ and $\lambda = 1$. Under these conditions we know that in the Newtonian limit when $D = D_0 \to 0$ (i.e., $\hbar \to 0$ or $m \to \infty$ but with mV finite) the particle undergoes a classical motion; for $D \neq 0$ the motion of the particle does not follow Newton's Laws any more due to its stochastic nature, but is governed by the more general equations

$$\frac{\partial\mathbf{v}}{\partial t} + \tfrac{1}{2}\nabla\mathbf{v}^2 = -\nabla\left[V - \tfrac{1}{2}\mathbf{u}^2 - \frac{\hbar}{2m}\nabla\cdot\mathbf{u}\right], \tag{34a}$$

$$\frac{\partial\mathbf{u}}{\partial t} + \nabla\left[\mathbf{v}\cdot\mathbf{u} + \frac{\hbar}{2m}\nabla\cdot\mathbf{v}\right] = 0, \tag{34b}$$

or, what is equivalent but simpler from the mathematical point of view, by the usual Schrödinger equation. A short digression seems justified here in order to clear up certain points. If, following some authors,[8,9] we look at Eq. (34a) from a Newtonian point of view taking $\mathbf{v}$ as the particle's velocity, we could say that the motion arises from two effective forces, the first due to the external potential $\mathbf{f}_0 = -\nabla V$ and the second being

$$\mathbf{a}_s = \mathfrak{D}_s\mathbf{u} = \nabla\left[\tfrac{1}{2}\mathbf{u}^2 + \frac{\hbar}{2m}\nabla\cdot\mathbf{u}\right],$$

which may be associated with the "potential" ϕ_B given by

$$\begin{aligned} \phi_B &= -\tfrac{1}{2}\mathbf{u}^2 - \frac{\hbar}{2m}\nabla\cdot\mathbf{u} \\ &= -\left(\frac{\hbar}{2m}\right)^2\left[\frac{\nabla^2\rho}{\rho} - \frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2\right], \end{aligned} \tag{34c}$$

where $\rho = \exp 2R = \psi^*\psi$. ϕ_B is just the "quantum-mechanical potential"[8] or Bohm's potential[9] and appears in Eq. (30a) added to V to give what was considered "an effective potential."[8] This point of view does not seem very convincing from the standpoint of the present theory, for firstly, the particle's

[8] D. Bohm, Phys. Rev. **85**, 166 (1952).
[9] R. J. Harvey, Phys. Rev. **152**, 1115 (1966).

velocity is not $\mathbf{v}$ but $\mathbf{c} = \mathbf{v} + \mathbf{u}$ and, secondly, it is possible to demonstrate (cf. Sec. IV) that in fact ϕ_B measures, in the average, the contribution of the stochastic velocity $\mathbf{u}$ to the total average kinetic energy. Furthermore, from (24) it follows that the total mean force is given in this case by $\mathbf{f} = \mathbf{f}_0 + 2\mathbf{a}_s$, i.e., the mean force generated by the interaction of the particle with the vacuum is given by $2\mathbf{a}_s$ and not by $\mathbf{a}_s$, while ϕ_B is associated with the latter. Hence, if we want to show explicitly the effective forces acting on the particle, we must rewrite Eqs. (34a) and (34b) in the following more symmetrical form:

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla[\tfrac{1}{2}(\mathbf{v}^2 + \mathbf{u}^2) + D\nabla \cdot \mathbf{u}] = -\nabla(V + 2\phi_B),$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla[\mathbf{v} \cdot \mathbf{u} + D\nabla \cdot \mathbf{v}] = 0.$$

It should be stressed that the theory developed up to this point does not give the value of D nor of the higher-order coefficients. For this we need a deeper understanding of the nature of the interaction between the quantum particle and the vacuum. The present theory is based only on the assumption that such an interaction exists and has a stochastic character. Thus, that D is a constant such that $D = \tilde{D}$ and has the value $\hbar/2m$ must be understood, presently, as an empirical result. An interesting attempt to understand theoretically this value has been given recently by de Broglie.[10]

IV. THE CONTINUITY AND ENERGY EQUATIONS. BROWNIAN MOTION

As mentioned, Eqs. (27) or rather their first integral equations (30), may be interpreted from the point of view of habitual stochastic theory by deriving from them a relation of the Fokker–Planck[6,7] type. For this purpose, let us rewrite (30) as

$$2D_0 \frac{\partial S}{\partial t} = -V + D_0\eta_-\nabla \cdot \mathbf{v} - \tfrac{1}{2}\mathbf{v}^2 + \lambda D_0\eta_+\nabla \cdot \mathbf{u} + \tfrac{1}{2}\lambda\mathbf{u}^2, \quad (35a)$$

$$2D_0 \frac{\partial R}{\partial t} = D_0\eta_-\nabla \cdot \mathbf{u} - \mathbf{v} \cdot \mathbf{u} - D_0\eta_+\nabla \cdot \mathbf{v}. \quad (35b)$$

The probability density ρ needed for our purpose is defined as before:

$$\rho = e^{2R} = \psi^*\psi. \quad (36)$$

With this definition, usual in quantum mechanics, (28b) gives

$$\mathbf{u} = \nabla(D_0 \ln \rho) = D_0 \frac{\nabla\rho}{\rho}. \quad (37)$$

[10] L. de Broglie, C. R. Acad. Sci. **264B**, 1041 (1967).

This is just the formula found by Einstein for the osmotic velocity in his elementary theory of Brownian motion.[11] Using (37), (35b) becomes

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{v}\rho - D_0\eta_-\nabla^2\rho = -\rho\left[D_0\eta_-\left(\frac{\nabla\rho}{\rho}\right)^2 + (\eta_+ - 1)\nabla \cdot \mathbf{v}\right]. \quad (38)$$

In the previous section we showed that ordinary quantum mechanics corresponds to setting $\eta_+ = 1$, $\eta_- = 0$. With these values, (38) reduces to the well-known continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{v}\rho = 0.$$

Here, as is to be expected, Eqs. (28) and (31) show that

$$\mathbf{v}\rho = -iD_0[\psi^*\nabla\psi - \psi\nabla\psi^*].$$

We may therefore reasonably consider (38) as the continuity equation for ρ, whatever the value of $\eta_\pm(t)$; this justifies the identification of ρ with the probability density for the ensemble underlying the theory. This ensemble may be defined as formed of all particles for which the mean value (in the restricted sense defined above) of the velocity and the energy (whose determination is discussed below) is the same. Equation (38) shows that any deviation of η_+ and η_- (and hence of D_+ and D_-) from their usual quantum-mechanical values implies the presence of sources for ρ which depend on ρ itself. It is possible to rewrite Eq. (38) in a slightly different form which corresponds more closely to that encountered in the theory of stochastic processes. For this purpose, let us introduce the relation $\mathbf{v} = \mathbf{c} - \mathbf{u}$ and use (37) once more to get, after minor rearrangements,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{c}\rho - D\nabla^2\rho = -(\eta - 1)\rho\left[\nabla \cdot \mathbf{c} + D_0\left(\frac{\nabla\rho}{\rho}\right)^2\right] - 2\eta_-\rho\left[\tfrac{1}{2}\nabla \cdot \mathbf{c} - D_0\nabla \cdot \frac{\nabla\rho}{\rho}\right], \quad (39)$$

where $\eta = D/D_0$ and $D = D_+ - D_-$, from (13). As before, for $D_+ = D_0$, $D_- = 0$, Eq. (39) becomes linear and source-free:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{c}\rho + D\nabla^2\rho. \quad (40)$$

Equation (40) is the Fokker–Planck equation of our problem in configuration space or, better, it is a

[11] A. Einstein, *The Theory of the Brownian Movement*, R. Fürth, Ed. (Dover Publications, Inc., New York, 1956).

particular case of a generalized Fokker–Planck–Kolmogorov equation of the type discussed by Pawula,[5] with $\mathbf{c}$ and D proportional to the first and second moments of the distribution in $\delta\mathbf{x}$, respectively, and the ratio of all other moments to Δt vanishing in the limit $\Delta t \to 0$. From it, we see that D plays the role of the diffusion coefficient. It is now clear that truncating the Taylor series, as was done above, is equivalent to stating *a priori* that all moments of order greater than two are of order $(\Delta t)^k$ with $k > 1$, so that in the limit $\Delta t \to 0$ the ratio of these moments to Δt vanish. This would appear to mean that the process is Markoffian, since for this type the higher coefficients do, indeed, vanish. It seems to us that this is a strong assumption that certainly requires experimental confirmation before being accepted.

Equation (40) corresponds simultaneously to ordinary quantum mechanics (it is an equivalent form of the continuity equation) and to the theory of Markoff processes in configuration space. From this point of view we have demonstrated that the usual quantum mechanics corresponds to a Markoff process.[12] Had we conserved higher terms in (27), Eq. (40) would become an equation with higher derivatives and the process would cease to be Markoffian; in this case, Schrödinger's equation would also contain higher derivatives, which, in turn, would imply a generalization of quantum mechanics to processes with "memory." Some qualitative comments about these questions are dealt with in next section.

If we are interested only in the asymptotic solutions of Eq. (40) for $t \to \infty$, we can greatly simplify things and recover the well-known Smoluchowski equation.[6] To see this, let us proceed first along the usual lines in the elementary theory of Brownian motion. Suppose that the particle moves in a medium which exerts on it a viscous force $-m\beta\mathbf{c}$ and a stochastic force of molecular origin $\mathbf{A}(t)$, with $\mathbf{A}(t)$ varying much more rapidly than $\mathbf{c}$. Then we may write the Langevin equation for the particle[6,7]:

$$m\frac{d\mathbf{c}}{dt} + m\beta\mathbf{c} = \mathbf{K} + \mathbf{A}(t),$$

where $\mathbf{K}$ is the external force. In the case $\beta t \gg 1$ the acceleration is so small that we can pass with enough accuracy to the static limit $d\mathbf{c}/dt = 0$, which means that we can write instead of $\mathbf{c}$ in Eq. (40) its approximate value $\mathbf{K}/m\beta$, because in the small time interval Δt, $\mathbf{c}$ and $\mathbf{K}$ may be considered constant, but

$$E\{\mathbf{A}(t)\} = 0.$$

Making use of this, Eq. (40) reduces to

$$\frac{\partial\rho}{\partial t} = -\nabla\cdot\frac{\mathbf{K}}{m\beta}\rho + D\nabla^2\rho,$$

which is precisely Smoluchowski's equation. Let us now look at this approximation in terms of our previous language, avoiding the use of Langevin's equation. The approximation consists in assuming that the total acceleration $\mathbf{a}$ is negligible, or, according to (18) and (24), that

$$\mathbf{f}_0 + (1+\lambda)\mathbf{a}_s = 0. \tag{41}$$

However, since $\mathbf{f}_0$ and $\mathbf{a}_s$ are linearly independent and $\mathbf{a}_s$ is not zero, (41) can be satisfied only if $\mathbf{f}_0 = 0$ and $\lambda = -1$ simultaneously. Furthermore, since both forces $\mathbf{K}$ and $-m\beta\mathbf{c}$ act on the particle, we have $m\mathbf{f}_0 = \mathbf{K} - m\beta\mathbf{c}$. In other words, the static approximation is achieved by setting

$$\mathbf{c} = \mathbf{K}/m\beta$$

and

$$\lambda = -1. \tag{42}$$

Thus we see that for $\beta t \gg 1$, Eq. (40) goes into Smoluchowski's equation. But we have also learned that for the Einstein–Smoluchowski treatment of Brownian motion we must set $\lambda = -1$, a value of λ which is different from its quantum-mechanical value; this implies that V_U in the Schrödinger equation for this problem is different from zero. In fact, for the free Brownian particle $D_+ = D$ is a constant which we can put equal to D_0 and $D_- = 0$ and hence Eq. (32) takes the form

$$2iD_0\frac{\partial\psi}{\partial t} = -2D^2\nabla^2\psi + 2[\tfrac{1}{2}\mathbf{u}^2 + D\nabla\cdot\mathbf{u}]\psi. \tag{43}$$

Equation (43), i.e., the Schrödinger equation for free Brownian motion in the Smoluchowski approximation, is nonlinear and, in general, more difficult to solve than the corresponding linear Smoluchowski (diffusion) equation. We see that, from this point of view, the free Brownian particle moves under the action of the "potential" V_U proportional to ϕ_B. The different values that the parameter λ takes in the two cases we have discussed, the quantum-mechanical one and the free Brownian motion in the Einstein–Smoluchowski approximation, point up the essentially different nature of the particle's interaction with its surroundings in the two cases, this interaction being frictionless in the first but dissipative in the second problem.

Let us now consider Eq. (35a). First note that if ρ vanishes at infinity, then the average of $\nabla\cdot\mathbf{u}$ may be

[12] For a direct demonstration, see L. de la Peña-Auerbach and A. M. Cetto, University of Mexico preprint (to be published).

written

$$D_0\langle\nabla\cdot u\rangle_{\mathrm{av}} = D_0^2\int\rho\nabla\cdot\frac{\nabla\rho}{\rho}\,dx$$
$$= -D_0^2\int\rho\left(\frac{\nabla\rho}{\rho}\right)^2 dx = -\langle\mathbf{u}^2\rangle_{\mathrm{av}}. \quad (44)$$

Introduce now Eq. (44) into the average of (35a):

$$\left\langle -2D_0\frac{\partial S}{\partial t}\right\rangle_{\mathrm{av}} = \langle\tfrac{1}{2}\mathbf{v}^2 + \tfrac{1}{2}\mathbf{u}^2 + V + \tfrac{1}{2}(\lambda-1)\mathbf{u}^2$$
$$+ \lambda(\eta_+ - 1)\mathbf{u}^2 - D_0\eta_-\nabla\cdot\mathbf{v}\rangle_{\mathrm{av}}. \quad (45)$$

This result may be interpreted as the energy law for our stochastic problem. In the quantum-mechanical case it reduces to

$$\left\langle -\hbar\frac{\partial S}{\partial t}\right\rangle_{\mathrm{av}} = \langle\tfrac{1}{2}m\mathbf{v}^2 + \tfrac{1}{2}m\mathbf{u}^2 + U\rangle_{\mathrm{av}},$$

which expresses that the average total energy is given by $\langle-\hbar(\partial S/\partial t)\rangle_{\mathrm{av}}$ and equals the sum of the average kinetic energy $\frac{1}{2}m\langle\mathbf{v}^2+\mathbf{u}^2\rangle_{\mathrm{av}}$ and the average potential energy $\langle U\rangle_{\mathrm{av}} = \langle mV\rangle_{\mathrm{av}}$. We see that the two velocities $\mathbf{v}$ and $\mathbf{u}$ contribute on an equal footing to the kinetic energy of the motion and that the kinetic energy of the stochastic velocity, $\frac{1}{2}m\langle\mathbf{u}^2\rangle_{\mathrm{av}}$, comes directly from the $\mathbf{u}$-terms in (35a), i.e., from Bohm's "potential"[3] [cf. Eq. (34c)]:

$$\langle m\phi_B\rangle_{\mathrm{av}} = -mD_0\langle\nabla\cdot\mathbf{u}\rangle_{\mathrm{av}} - \tfrac{1}{2}m\langle\mathbf{u}^2\rangle_{\mathrm{av}}$$
$$= \tfrac{1}{2}m\langle\mathbf{u}^2\rangle_{\mathrm{av}},$$

where we have used once more Eq. (44). As we have seen, the average total energy is given by

$$\epsilon = \left\langle -2D_0 m\frac{\partial S}{\partial t}\right\rangle_{\mathrm{av}}. \quad (46)$$

Defining the expectation value $\langle\hat{\epsilon}\rangle$ of an operator $\hat{\epsilon}$ by

$$\langle\hat{\epsilon}\rangle = \int\psi^*\hat{\epsilon}\psi\,d\mathbf{x},$$

as is usual in quantum mechanics, we get immediately that the expectation value of the operator

$$\hat{\epsilon} = 2iD_0 m\frac{\partial}{\partial t} \quad (47)$$

is equal to the average energy ϵ; therefore we can call $\hat{\epsilon}$ the energy operator. In an entirely similar way, it is possible to introduce the momentum operator.[2,3] To see this, first note that from (36) and (37) it follows, as it must be, that

$$\langle\mathbf{u}\rangle = \langle\mathbf{u}\rangle_{\mathrm{av}} = 0. \quad (48)$$

Now, from the gradient of Eq. (31) and Eqs. (28) and (48) we get that

$$\langle -2iD_0\nabla\rangle = \langle\mathbf{v}\rangle_{\mathrm{av}} = \langle\mathbf{c}\rangle_{\mathrm{av}}$$

and, therefore, that the momentum operator $\hat{\mathbf{p}}$, such that $\langle\hat{\mathbf{p}}\rangle = \langle m\mathbf{c}\rangle_{\mathrm{av}}$, is given by

$$\hat{\mathbf{p}} = -2iD_0 m\nabla. \quad (49)$$

It should be noted that Eqs. (47) and (49) generalize the concept of energy and momentum operators to stochastic processes of the type discussed in this section. Clearly, for the quantum-mechanical case when $D_0 = \hbar/2m$, they reduce to their usual values $\hat{\epsilon} = i\hbar(\partial/\partial t)$ and $\hat{\mathbf{p}} = -i\hbar\nabla$. As is well known, the uncertainty relations for $(\hat{p}, x)$ and $(t, \hat{\epsilon})$ follow immediately from the above results and are thus a consequence and in some sense also a measure of the stochastic properties of the ensemble. For example, if we introduce the velocity operator $\hat{\mathbf{c}} = \hat{\mathbf{p}}/m$, such that $\langle\hat{\mathbf{c}}\rangle = \langle\mathbf{c}\rangle_{\mathrm{av}}$ and $\langle\hat{\mathbf{c}}^2\rangle = \langle\mathbf{v}^2+\mathbf{u}^2\rangle_{\mathrm{av}}$, then we have when $D = D_0$,

$$\langle(\Delta x_i)^2\rangle\langle(\Delta c_i)^2\rangle \geq D_0^2 = \frac{1}{4}\left[\lim_{\Delta t\to 0}\frac{1}{\Delta t}E\{(\delta x_i)^2\}\right]^2$$

where

$$\Delta x_i = x_i - \langle x_i\rangle_{\mathrm{av}}, \quad \Delta c_i = c_i - \langle c_i\rangle_{\mathrm{av}},$$

and

$$\delta x_i = x_i(t+\Delta t) - x_i(t).$$

We see that the dispersion of an individual particle, owing to its interaction with the vacuum, sets a lower limit to the product of the fluctuations of x_i and c_i in the ensemble.

V. COMMENTS ON THE POSSIBLE HIGHER-ORDER EFFECTS

For the study of some possible effects of the higher-order terms and for simplicity in the writing, we introduce the following conventions. Firstly, all the quantities written before to second order will carry here the superscript 0; secondly, the higher-order terms will be written in shorthand notation as follows:

$$\sum_{ijk\cdots} F_n^{ijk\cdots}\partial_i\partial_j\partial_k\cdots = F_n\partial^{(n)}, \quad (50a)$$

where $F_n^{ijk\cdots}$ is the $ijk\cdots$-component of the coefficient of order n in the Taylor series (6), for $n > 2$. Also we write

$$\sum_{n=3}^{\infty} F_n\partial^{(n)} = F_n\partial^n. \quad (50b)$$

With these conventions, Eqs. (8) take the form

$$\mathfrak{D} = \mathfrak{D}^0 + F_n\partial^n,$$
$$\tilde{\mathfrak{D}} = \tilde{\mathfrak{D}}^0 + \tilde{F}_n\partial^n. \quad (51)$$

Then, extending the notation of Eq. (13) to the

higher-order terms, we write

$$F_n^+ = \tfrac{1}{2}(\tilde{F}_n + F_n),$$
$$F_n^- = \tfrac{1}{2}(\tilde{F}_n - F_n), \tag{52}$$

and hence from (11) we get

$$\mathfrak{D}_c = \mathfrak{D}_c^0 - F_n^- \partial^n,$$
$$\mathfrak{D}_s = \mathfrak{D}_s^0 + F_n^+ \partial^n. \tag{53}$$

Introduce now these operators into the fundamental equations (17) and from them, using the method of Sec. III assuming that $F_n^{\pm}$ do not depend on the coordinates, obtain the corresponding Schrödinger equation. The result, for $D_+ = D$, $D_- = 0$, $\lambda = +1$, is

$$2iD\frac{\partial \psi}{\partial t} = -2D^2\nabla^2\psi + V\psi + V_S\psi, \tag{54}$$

where V_S is given by

$$V_S = -2D\sum_{n=3}^{\infty} F_{cn}\partial^{(n)} \ln \psi \equiv \sum_{n=3}^{\infty} V_S^{(n)}, \tag{55}$$

with

$$F_{cn} = F_n^+ - iF_n^-. \tag{56}$$

Equation (54) is the form Schrödinger's equation takes when we eliminate the assumption made in Secs. II and IV, namely, that all F_n are zero, i.e., when we no longer assume that the stochastic interaction of the particle with its surroundings is Markoffian, but corresponds to a more general process with some "memory." We see that the nonvanishing higher-order terms give rise to a "potential" V_S, which depends on both velocities v and u and their derivatives through the derivatives of $\ln \psi = R + iS$. The question whether the coefficients F_n are zero (as was assumed in Secs. III and IV) or different from zero (as we here assume) remains open as long as we do not have a theory of the interaction between the particle and the surrounding medium; this lack of information makes it impossible at the time being to get quantitative conclusions from Eq. (54), because it involves V_S, i.e., depends on the still unknown parameters $F_n^{\pm}$. Nevertheless, it seems interesting to investigate a little further some qualitative implications of Eq. (54) for simple cases, at least to see if the introduction of the coefficients F_n may make any sense.

Restricting ourselves to this scope, let us treat V_S as a small perturbation and study what is almost the simplest problem we can handle: the corrections to the energy levels of a stationary system to first order in perturbation theory, assuming that $F_3^{\pm}$ are zero (because of isotropy) and F_4^- is zero, but $F_4^{+ijkl} = F_4\delta_{ij}\delta_{kl}$ with F_4 a constant (in analogy with $D_{ij}^{\pm}$) and that all the remaining coefficients $F_n^{\pm}$ may be neglected in a first-order calculation. Then we can write $V_S = V_4$ or

$$V_S = -2DF_4\nabla^2\nabla^2 \ln \psi. \tag{57}$$

The correlation δE to the energy levels of a stationary system to first-order in perturbation theory due to V_S as given by Eq. (57) may be obtained by a straightforward but a little lengthy calculation. The result may be written as follows:

$$\frac{\delta E}{m} = \langle V_S \rangle = -2D^{-1}F_4\langle \nabla^2 V \rangle + D^{-3}F_4\langle (\tfrac{1}{2}m\mathbf{u}^2 + mV - E)^2 \rangle. \tag{58}$$

Since this δE is not identically zero for $F_4 \neq 0$, the conclusion is that we may expect a small shift of the energy levels of a stationary system if some of the higher-order coefficients do not vanish. Clearly, if in fact this δE corresponds to a real effect, it must be very small, because we know that the Schrödinger equation, which corresponds to putting $F_n = 0$, is an excellent approximation for nonrelativistic spinless systems. That this correction is indeed small can be seen from the following argument. It is well known that the radiative corrections in quantum electrodynamics give rise to a term proportional to $\langle \nabla^2 V \rangle$, which is responsible for the most important contribution to the Lamb shift.[13] Suppose one could identify the corresponding term in Eq. (58) as a contribution to the Lamb shift; then, F_4 must be at most of order

$$F_4 \sim \alpha c \lambda_c^3, \tag{59}$$

where α is the fine-structure constant, c the velocity of light, and λ_c the Compton wave-length. If F_4 exceeds this value, then we would be predicting a correction which does not exist. Nevertheless, the result is encouraging, since it shows that further developments of the theory may yield interesting results.[14] This will be particularly so for its extension to relativistic particles with spin, because our arguments, while suggestive, cannot be made conclusive until either a value is found for F_4 from first principles or at least a relation is established between the prediction for δE and that for some other effect, e.g., the anomalous magnetic moment. Work on this extension is being carried out at present.

VI. CONCLUSIONS

We have reformulated the theory of stochastic processes as a generalization of Newtonian mechanics

[13] J. M. Jauch and F. Rohrlich, *The Theory of Photons and Electrons* (Addison-Wesley Publ. Co., Reading, Mass., 1955).

[14] It is worth noting that there exist semi-classical explanations of the Lamb shift for nonrelativistic electrons, thus showing that it is not wholly a relativistic effect. For example, T. A. Welton, Phys. Rev. 74, 1157 (1948).

and shown that Schrödinger's equation emerges from this theory as a particular case, which, incidentally, is the simplest possible from a certain mathematical point of view. If together with the amplitude ψ previously introduced for mathematical reasons we introduce the quantity $\rho = \psi^*\psi$, then the theory produces a Fokker–Planck equation in configuration space for ρ, showing that ρ must be interpreted as a probability density and hence ψ as a probability amplitude. The Fokker–Planck equation may be written alternatively in the form of the usual continuity equation of quantum mechanics, thus identifying ρ with the probability density of quantum mechanics. Furthermore, the usual quantum-mechanical operators and commutation relations emerge from the theory in a simple and direct way, as a consequence of the stochastic nature of the motion. In this way we have demonstrated that it is possible, at least in principle, to reinterpret ordinary nonrelativistic quantum mechanics as a stochastic process characterized by certain values of the parameters of the general theory, some of these values differing from those needed to describe Brownian motion. We interpret this difference in the parameters as a manifestation of the different mechanisms responsible for the interaction between the particle and the medium through which it moves.

With the methods here developed we have, in principle, three ways to deal with stochastic and quantum problems: starting from the basic equations given in Sec. II, which represents the Newtonian approach, so to speak; writing a Schrödinger equation for the problem; or, finally, starting with the corresponding Fokker–Planck and energy equations given in Sec. IV, a method which may be compared with hydrodynamics. In practice, however, the mathematical structure of the equations seems to indicate that in every case the methods usually employed are the most appropriate, even though the theory gives a Schrödinger equation for Brownian problems and a Fokker–Planck equation for quantum-mechanical problems.

From the standpoint of the results here presented usual quantum mechanics corresponds to a Markoff process with all the moments of order higher than two vanishing in the limit $\Delta t \to 0$ more strongly than Δt. If we consider this only as an approximation and retain the remaining moments in the equations, then the higher-order moments introduce more terms in the Schrödinger equation, giving rise to a perturbing potential; in other words, memory terms appear in the equations, the process ceasing to be Markoffian. These non-Markoffian terms may produce in the general case a shift of the energy levels; as an example, the fourth-order moment introduces a correction to the energy levels of the hydrogen-like atom, which has just the form of the dominating correction responsible for the Lamb shift in quantum electrodynamics. The calculation of the perturbation due to the additional terms is only qualitative at present because we lack a theory capable of predicting the value of the moments, but we may expect that a more thorough study of the problem may be of value to get a definitive conclusion about these questions.

The interest of the theory seems to be twofold. On the one hand, it allows us to reinterpret quantum mechanics from a different, clear, and simple physical point of view. On the other hand, we expect the theory to yield useful results in going beyond the domain of present-day quantum mechanics. Work along these lines is being carried out and will be reported on in due course.

ACKNOWLEDGMENTS

The author wishes to express his gratitude to T. A. Brody and L. García-Colín for very valuable discussions and critical reading of the manuscript, and to thank E. Piña for interesting discussions.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Potentials for Three-Body Systems

R. C. WHITTEN
NASA-Ames Research Center, Space Sciences Division, Moffett Field, California

(Received 22 July 1968)

Simple expressions for the Coulomb, Gaussian, and harmonic-oscillator potentials acting between pairs of particles in a three-body system are developed. Each expression consists of an expansion in the S-wave generalized angular-momentum eigenfunctions for three particles.

I. INTRODUCTION

The quantum mechanics of three-body systems has received a great deal of attention recently by a number of investigators.[1–6] These investigations have been concerned with the kinematic representations of three particles, as well as with applications to specific problems. Several different coordinate systems have been proposed, but that originally suggested by Smith[2] is particularly well adapted to the treatment of some systems. It is the purpose of this paper to present expressions of particularly simple form for the Coulomb, Gaussian, and harmonic-oscillator potentials in terms of Smith's coordinates.

All coordinate systems which have been suggested so far separate the motion of the center of mass (three independent coordinates) from the relative motion of the particles (six independent coordinates). The latter are represented by the two vectors $\boldsymbol{\xi}^1$ and $\boldsymbol{\xi}^2$ illustrated in Fig. 1. They are related to the position vectors $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3$ in the "space-fixed" system by the relations[1]

$$\boldsymbol{\xi}^1 = (1/d)(\mathbf{r}^2 - \mathbf{r}^1), \tag{1}$$

$$\boldsymbol{\xi}^2 = d\left(\mathbf{r}^3 - \frac{m_1\mathbf{r}^1 + m_2\mathbf{r}^2}{m_1 + m_2}\right), \tag{2}$$

where

$$d^2 = \frac{m_3}{\mu}\left(\frac{m_1 + m_2}{m_1 + m_2 + m_3}\right) \tag{3}$$

and μ is the reduced mass

$$\mu^2 = \frac{m_1m_2m_3}{m_1 + m_2 + m_3}. \tag{4}$$

The relative motion consists of the motion of three particles within the "body-fixed" axes and the rotation of the latter with respect to "space-fixed" axes. Such a rotation is conveniently expressed by the Euler angles α, β, γ, which are also illustrated in the figure. It is immediately obvious that velocity-independent central potentials are not functions of the Euler angles. The coordinates in the body-fixed system, $\bar{\boldsymbol{\xi}}^1$ and $\bar{\boldsymbol{\xi}}^2$, are expressed in terms of a hyperradius ρ and two "kinematic" angles Θ and Φ by the relations[2]

$$\begin{aligned}
\bar{\xi}^1_1 &= \rho\cos\Theta\cos\Phi,\\
\bar{\xi}^1_2 &= -\rho\sin\Theta\sin\Phi,\\
\bar{\xi}^1_3 &= 0,\\
\bar{\xi}^2_1 &= \rho\cos\Theta\sin\Phi,\\
\bar{\xi}^2_2 &= \rho\sin\Theta\cos\Phi,\\
\bar{\xi}^2_3 &= 0,\\
\rho &= [|\boldsymbol{\xi}^1|^2 + |\boldsymbol{\xi}^2|^2]^{\frac{1}{2}},
\end{aligned} \tag{5}$$

in which the subscripts 1, 2, and 3 refer to the "x," "y," and "z" components, respectively. The coordinates $\bar{\boldsymbol{\xi}}^1$, $\bar{\boldsymbol{\xi}}^2$ are first transformed to the irreducible or spherical representation in which

$$\begin{aligned}
\bar{\xi}^j_{\pm1} &= (2)^{-\frac{1}{2}}(\mp\bar{\xi}^j_1 - i\bar{\xi}^j_2),\\
\bar{\xi}^j_0 &= \bar{\xi}^j_3.
\end{aligned} \tag{6}$$

The irreducible form of the $\bar{\xi}^1$, $\bar{\xi}^2$ is then transformed to the equivalent representation in the space-fixed system $\boldsymbol{\xi}^1$, $\boldsymbol{\xi}^2$ by the relation

$$\xi^i_j = \sum_{k=0,\pm1} \bar{\xi}^i_k D^1_{jk}(\alpha\beta\gamma), \tag{7}$$

in which the D^1 is the three-dimensional representation of the rotation group $O(3)$. The definition of the D^l given by Edmonds[7] is used throughout this paper.

II. THE SCHRÖDINGER EQUATION AND THE GENERALIZED ANGULAR-MOMENTUM OPERATOR

In this section we digress slightly from the main theme in order to build a rationale for our treatment of the potentials. The Schrödinger equation for three particles in the center-of-mass system[1] can be written as

$$\left(\sum_{i=1}^{2}\sum_{j=1}^{3}\frac{\partial^2}{\partial(\xi^i_j)^2} + \frac{2\mu}{\hbar^2}(E - V)\right)\psi = 0, \tag{8}$$

[1] F. T. Smith, Phys. Rev. **120**, 1058 (1960).
[2] F. T. Smith, J. Math. Phys. **3**, 735 (1962).
[3] R. C. Whitten and F. T. Smith, J. Math. Phys. **9**, 1103 (1968).
[4] W. Zickendraht, Ann. Phys. (N.Y.) **35**, 18 (1965).
[5] A. J. Dragt, J. Math. Phys. **6**, 533 (1965).
[6] A. K. Bhatia and A. Temkin, Rev. Mod. Phys. **36**, 1050 (1964).
[7] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, N.J., 1957).

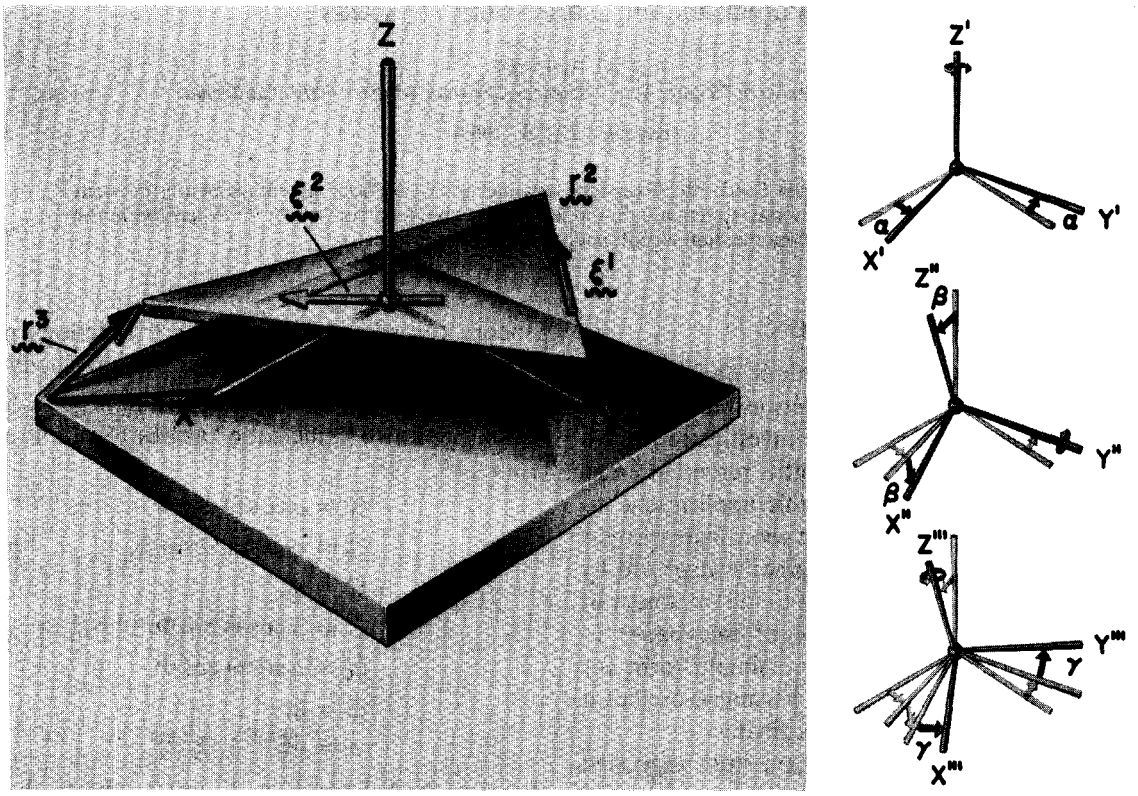


FIG. 1. The coordinate system for three particles; x, y, z represent the space-fixed axes; x''', y''', z''' represent the body-fixed system. The Euler angles of the principal are represented by α, β, γ.

where E is the energy and V is the potential energy operator. This form of the equation is not a convenient one for most purposes, so we recast it to

$$\left[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right) - \frac{\Lambda^2}{\rho^2} + \frac{2\mu}{\hbar^2}(E - V)\right]\psi = 0, \quad (9)$$

where Λ^2 is the generalized angular-momentum (GAM) scalar operator[8]

$$\Lambda^2 = \frac{1}{\sin 4\Theta}\frac{\partial}{\partial\Theta}\sin 4\Theta\frac{\partial}{\partial\Theta} + \frac{1}{\cos^2 2\Theta}\left(\frac{\partial^2}{\partial\Phi^2} + \frac{\partial^2}{\partial\gamma^2} - \frac{\partial^2}{\partial\Phi\partial\gamma}\sin 2\Theta\right) - \frac{2}{\sin^2 2\Theta}\left(L^2 + \frac{\partial^2}{\partial\gamma^2}\right) + 2\frac{\cos 2\Theta}{\sin^2 2\Theta}(L_{+1}^2 + L_{-1}^2). \quad (10)$$

Here, L^2 is the orbital angular-momentum operator with eigenvalues $l(l+1)$ (l integer ≥ 0) and L_{+1} and L_{-1} are the familiar ladder operators of orbital angular momentum. Λ^2 has the eigenvalues $\lambda(\lambda+4)$, where $\lambda = 0, 2, 4, 6\cdots$ or $1, 3, 5\cdots$. In addition to Λ^2, we also have the commuting observable

$$\sum_i = -\frac{\partial^2}{\partial\Phi^2}, \quad (11)$$

whose eigenvalues are[4]

$$\sigma = 0, \pm 2, \pm 4\begin{cases}\cdots \pm\lambda, & \text{if } \lambda \text{ is even and } L \text{ is even,}\\ \cdots \pm(\lambda-2), & \text{if } \lambda \text{ is even and } L \text{ is odd,}\end{cases}$$

or

$$\sigma = \pm 1, \pm 3, \pm 5\begin{cases}\cdots \pm\lambda, & \text{if } \lambda \text{ is odd and } L \text{ is odd,}\\ \cdots \pm(\lambda-2), & \text{if } \lambda \text{ is odd and } L \text{ is even.}\end{cases}$$

Finally, there is a second Casimir operator[2,3] $\sum_d$ which need not concern us here. The observables E, Λ^2, $\sum_i \sum_d$, L^2, and

$$L_0 = -\frac{\partial^2}{\partial\alpha^2} \quad (12)$$

completely specify the system. In the particularly simple case where $L^2\psi = 0$ (S states), the GAM

[8] Λ^2 is a Casimir operator for the group $SU(4)$. See Refs. 3 and 5.

equation

$$\Lambda^2\psi = \lambda(\lambda+4)\psi \tag{13}$$

takes the form

$$\left[\frac{1}{\sin 4\Theta}\frac{\partial}{\partial\Theta}\sin 4\Theta\frac{\partial}{\partial\Theta} - \frac{2\sigma^2}{(1+\cos 4\Theta)} - \lambda(\lambda+4)\right]\psi = 0. \tag{14}$$

Its solutions are the diagonal elements of the $(\frac{1}{2}\lambda+1)$-dimensional representation of $SU(2)$:

$$\psi = \mathfrak{D}^{\frac{1}{2}\lambda}_{\frac{1}{2}\sigma\frac{1}{2}\sigma}(4\Phi, 4\Theta, 0), \tag{15}$$

where λ and σ must, of course, be even; script type is used to denote kinematic rotations, italic type to denote spatial rotations. It can be shown[4] that the appropriate interval of integration with respect to Θ is 0 to $\pi/4$, and with respect to Φ is 0 to $\pi/2$ so that 4Φ, 4Θ are appropriate arguments for all the eigenfunctions of Λ^2. Hence, we seek to expand the potential V in a series of functions which are orthogonal on this interval. In particular, we shall see that the functions of the expansion contain GAM S-state functions.

III. THE POTENTIAL EXPANSIONS

If the interactions are central two-body forces, one can always write the potential operator as

$$V = V(|\mathbf{r}^3-\mathbf{r}^2|, |\mathbf{r}^3-\mathbf{r}^1|, |\mathbf{r}^2-\mathbf{r}^1|). \tag{16}$$

In particular, the Coulomb potential between a particle i of charge e and another j of charge eZ is

$$V^c_{ij} = e^2Z/|\mathbf{r}^i-\mathbf{r}^j|. \tag{17}$$

From Eqs. (1) and (2) we can express the position vectors $\mathbf{r}^j-\mathbf{r}^i$ in terms of $\boldsymbol{\xi}^i$ as

$$\mathbf{r}^2-\mathbf{r}^1 = d\boldsymbol{\xi}^1, \tag{18}$$

$$\mathbf{r}^3-\mathbf{r}^1 = \frac{1}{d}\left[\boldsymbol{\xi}^2 + \frac{m_2d^2}{m_1+m_2}\boldsymbol{\xi}^1\right], \tag{19}$$

$$\mathbf{r}^3-\mathbf{r}^2 = \frac{1}{d}\left[\boldsymbol{\xi}^2 - \frac{m_1d^2}{m_1+m_2}\boldsymbol{\xi}^1\right]. \tag{20}$$

The corresponding distances become[4]

$$|\mathbf{r}^i-\mathbf{r}^j| = \rho c_k[1+\cos 2\Theta\cos 2(\Phi+\delta_k)]^{\frac{1}{2}}, \quad i,j,k \text{ cyclic}, \tag{21}$$

$$\begin{aligned} c_k &= d(2)^{-\frac{1}{2}}, && \text{if } k=3,\\ &= \frac{d}{\sqrt{2}}\left[\frac{1}{d^4}+\left(\frac{m_1}{m_1+m_2}\right)^2\right]^{\frac{1}{2}}, && \text{if } k=1,\\ &= \frac{d}{\sqrt{2}}\left[\frac{1}{d^4}+\left(\frac{m_2}{m_1+m_2}\right)^2\right]^{\frac{1}{2}}, && \text{if } k=2, \end{aligned} \tag{22}$$

$$\begin{aligned} \sin 2\delta_k &= \frac{2m_3}{d^2(m_2+m_3)}, && \text{if } k=1,\\ &= \frac{-2m_3}{d^2(m_1+m_3)}, && \text{if } k=2,\\ &= 0, && \text{if } k=3. \end{aligned} \tag{23}$$

We now wish to find an expansion of

$$[1+\cos 2\Theta\cos 2(\Phi+\delta_k)]^{-\frac{1}{2}}.$$

It is immediately apparent that this expression can be recast as

$$\begin{aligned} &[1+\tfrac{1}{2}\cos 2\Theta(e^{2i(\Phi+\delta_k)}+e^{-2i(\Phi+\delta_k)})]^{-\frac{1}{2}}\\ &\quad= [1+\tfrac{1}{2}\mathfrak{D}^{\frac{1}{2}}_{\frac{1}{2}\frac{1}{2}}(4\Phi+4\delta_k, 4\Theta, 0)\\ &\qquad+\tfrac{1}{2}\mathfrak{D}^{\frac{1}{2}}_{-\frac{1}{2}-\frac{1}{2}}(4\Phi+4\delta_k, 4\Theta, 0)]^{-\frac{1}{2}}, \end{aligned} \tag{24}$$

which still does not help us very much. However, with the aid of the binomial theorem, we obtain the following series (where the arguments are omitted from the $\mathfrak{D}$'s):

$$\begin{aligned} &[1+\tfrac{1}{2}\mathfrak{D}^{\frac{1}{2}}_{\frac{1}{2}\frac{1}{2}}+\tfrac{1}{2}\mathfrak{D}^{\frac{1}{2}}_{-\frac{1}{2}-\frac{1}{2}}]^{-\frac{1}{2}}\\ &\quad=\sum_{\nu=0}^{\infty}\binom{-\frac{1}{2}}{\nu}\left(\frac{1}{2}\right)^{\nu}\sum_{\mu=0}^{\nu}\binom{\nu}{\mu}\mathfrak{D}^{\frac{1}{2}(\nu-\mu)}_{\frac{1}{2}(\nu-\mu),\frac{1}{2}(\nu-\mu)}\mathfrak{D}^{\frac{1}{2}\mu}_{-\frac{1}{2}\mu,-\frac{1}{2}\mu}. \end{aligned} \tag{25}$$

The group properties of the $\mathfrak{D}$'s can be invoked to obtain a great simplification. Upon expansion in the appropriate Clebsch–Gordan series,[7] the terms on the right-hand side of Eq. (25) are expressed as

$$\begin{aligned} &\binom{\nu}{\mu}\mathfrak{D}^{\frac{1}{2}(\nu-\mu)}_{\frac{1}{2}(\nu-\mu),\frac{1}{2}(\nu-\mu)}\mathfrak{D}^{\frac{1}{2}\mu}_{-\frac{1}{2}\mu,-\frac{1}{2}\mu}\\ &\quad=\binom{\nu}{\mu}\sum_{r=|\nu-2\mu|}^{\nu}\left(C^{\frac{1}{2}(\nu-\mu),\frac{1}{2}\mu,\frac{1}{2}r}_{\frac{1}{2}(\nu-\mu),\frac{1}{2}\mu,\frac{1}{2}\nu-\mu}\right)^2\mathfrak{D}^{\frac{1}{2}r}_{\frac{1}{2}\nu-\mu,\frac{1}{2}\nu-\mu}\\ &\quad=\sum_r\frac{(r+1)\nu!}{(\frac{1}{2}(\nu-r))!\,(\frac{1}{2}(\nu+r+1))!}\mathfrak{D}^{\frac{1}{2}r}_{\frac{1}{2}\nu-\mu,\frac{1}{2}\nu-\mu}, \end{aligned} \tag{26}$$

where we have used the relation[7]

$$C^{\frac{1}{2}(\nu-\mu),\frac{1}{2}\mu,\frac{1}{2}r}_{\frac{1}{2}(\nu-\mu),-\frac{1}{2}\mu,\frac{1}{2}\nu-\mu} = \left[\frac{(r+1)(\nu+r)!\,\mu!}{(\frac{1}{2}(\nu-r))!\,(\frac{1}{2}(\nu+r)+1)!}\right] \tag{27}$$

for the Clebsch–Gordan coefficients. Hence, the expansion of expression (26) becomes

$$\sum_{\nu=0}^{\infty}\sum_{r,u}(r+1)\times\frac{\Gamma(\nu+\frac{1}{2})(-\frac{1}{2})^{\nu}}{\Gamma(\frac{1}{2})(\frac{1}{2}(\nu-r))!\,(\frac{1}{2}(\nu+r)+1)!}\mathfrak{D}^{\frac{1}{2}r}_{\frac{1}{2}\nu-\mu,\frac{1}{2}\nu-\mu}, \tag{28}$$

where r and ν have the same parity because of the properties of the $\mathfrak{D}$'s. Replacing $\frac{1}{2}\nu-\mu$ by μ and redefining the dummy index ν such that $\nu\to\nu+r$,

we obtain

$$\sum_{\nu=0}^{\infty}\sum_{r,u}(r+1)\frac{\Gamma(2\nu+r+\frac{1}{2})}{\Gamma(\frac{1}{2})\nu!\,(\nu+r+1)!}(-\tfrac{1}{2})^{2\nu+r}\mathfrak{D}^{\frac{1}{2}r}_{\frac{1}{2}\mu\frac{1}{2}\mu}. \tag{29}$$

We now employ the duplication theorem for gamma functions[9]

$$\Gamma(2\nu+r+\tfrac{1}{2})=\Gamma\left(\nu+\frac{2r+1}{4}\right)\Gamma\left(\nu+\frac{2r+3}{4}\right)\frac{2^{2\nu+r}}{(2\pi)^{\frac{1}{2}}} \tag{30}$$

and interchange the order of summation over ν and r. This is permissible if the series is absolutely convergent[10] when summed over ν or r for $|\mathfrak{D}^{\frac{1}{2}r}_{\frac{1}{2}\mu\frac{1}{2}\mu}|<1$. Such may be shown to be the case. Carrying out the summation over ν yields

$$\begin{aligned}\sum_{\nu=0}^{\infty}&\frac{\Gamma(\nu+\frac{1}{4}(2r+1))\Gamma(\nu+\frac{1}{4}(2r+3))}{\nu!\,(\nu+r+1)!}\\&=\frac{\Gamma(\frac{1}{4}(2r+1))\Gamma(\frac{1}{4}(2r+3))}{\Gamma(r+2)}\\&\quad\times{}_2F_1\left[\frac{2r+1}{4},\frac{2r+3}{4};r+2;1\right]\\&=\frac{\Gamma(\frac{1}{4}(2r+1))\Gamma(\frac{1}{4}(2r+3))}{\Gamma(\frac{1}{4}(2r+5))\Gamma(\frac{1}{4}(2r+7))}\\&=\frac{16}{(2r+1)(2r+3)},\end{aligned} \tag{31}$$

where ${}_2F_1$ is a hypergeometric function. Hence, we can express the expansion as

$$V^c_{ij}=\frac{16}{\rho(2\pi)^{\frac{1}{2}}}\sum_{r=0}^{\infty}\frac{(r+1)(-1)^r}{(2r+1)(2r+3)}\sum_{\mu=-r}^{r}\mathfrak{D}^{\frac{1}{2}r}_{\frac{1}{2}\mu\frac{1}{2}\mu}, \tag{32}$$

which is our final very simple result. It will be recalled that the $\mathfrak{D}^{\frac{1}{2}r}_{\frac{1}{2}\mu\frac{1}{2}\mu}$ are S state eigenfunctions of the GAM operator.

It is immediately obvious that the technique outlined in this section can be applied to potentials other than the Coulomb. For example, the Gaussian potential

$$V^G_{ij}=a\exp(K|\mathbf{r}^i-\mathbf{r}^j|^2) \tag{33}$$

has the expansion

$$\begin{aligned}V^G_{ij}&=a\frac{2\exp(-Kc_k^2\rho^2)}{Kc_k^2\rho^k}\\&\quad\times\sum_{r=0}^{\infty}(-1)^r(r+1)I_{r+1}(Kc_k^2\rho^2)\sum_{\mu}\mathfrak{D}^{\frac{1}{2}r}_{\frac{1}{2}\mu\frac{1}{2}\mu}\end{aligned} \tag{34}$$

[$I_{r+1}(x)$ is the modified Bessel function], and the harmonic-oscillator potential

$$V^H_{ij}=\tfrac{1}{2}\omega_{ij}(\mathbf{r}^i-\mathbf{r}^i_0-\mathbf{r}^j+\mathbf{r}^j_0)^2, \tag{35}$$

where $\mathbf{r}^i_0$ and $\mathbf{r}^j_0$ are the equilibrium positions of particles i and j, has the expansion

$$\begin{aligned}V^H_{ij}=\frac{\omega_{ij}}{2}\rho^2(c_k)^2[1&+\tfrac{1}{2}\mathfrak{D}^{\frac{1}{2}}_{\frac{1}{2}\frac{1}{2}}(4(\Phi+\delta_k),4\Theta,0)\\&+\tfrac{1}{2}\mathfrak{D}^{\frac{1}{2}}_{-\frac{1}{2}-\frac{1}{2}}(4(\Phi+\delta_k),4\Theta,0)],\\\rho^2=|\xi^1-\xi^1_0|^2&+|\xi^2-\xi^2_0|^2.\end{aligned} \tag{36}$$

IV. APPLICATION

As an application of the Coulomb-potential expansion given above, let us consider the case where the S-state eigenfunction of the system is written as

$$\psi=\sum_{\lambda\sigma}a^{\lambda}_{\sigma}R_{\lambda}(\rho)\mathfrak{D}^{\frac{1}{2}\lambda}_{\frac{1}{2}\sigma\frac{1}{2}\sigma}(4\Phi,4\Theta,0). \tag{37}$$

The quantities which must be derived in this case are the scalar products $(\mathfrak{D}^{\frac{1}{2}\lambda'}_{\frac{1}{2}\sigma'\frac{1}{2}\sigma'},V\mathfrak{D}^{\frac{1}{2}\lambda}_{\frac{1}{2}\sigma\frac{1}{2}\sigma})$. For example, in the case of the helium atom or the negative ion of hydrogen,

$$\begin{aligned}&(\mathfrak{D}^{\frac{1}{2}\lambda'}_{\frac{1}{2}\sigma'\sigma\frac{1}{2}'},V\mathfrak{D}^{\frac{1}{2}\lambda}_{\frac{1}{2}\sigma\frac{1}{2}\sigma})\\&=\frac{64}{\rho(2)^{\frac{1}{2}}}e^2\sum_{r=\frac{1}{2}|\lambda'-\lambda|}^{\frac{1}{2}(\lambda'+\lambda)}\frac{(-1)^r[2\sqrt{2}\,Z\cos(\frac{1}{4}(\sigma-\sigma')\pi)-1]}{(2r+1)(2r+3)}\\&\qquad\times(C^{\frac{1}{2}\lambda,\frac{1}{2}\lambda',\frac{1}{2}r}_{\frac{1}{4}\sigma,-\frac{1}{4}\sigma',\frac{1}{4}(\sigma-\sigma')})^2,\end{aligned} \tag{38}$$

where Z is the atomic number. Substitution of Eq. (37) into the Schrödinger equation (9) and application of Eq. (38) yields a set of coupled hyperradial equations whose solutions (with boundary conditions applied) suggest hydrogenic type functions

$$R_{\lambda}(x)=e^{-\frac{1}{2}x}x^{\lambda}L^{2\lambda+4}_n(x), \tag{39}$$

where n is an integer. Use of the orthogonality properties of R_{λ} and proper symmetrization of the wavefunctions will yield a coupled set of algebraic equations (infinite in number) which can be solved on a computer by suitably truncating the series (37). Similar programs can be carried out for other potentials which are expandable in the above manner.

ACKNOWLEDGMENTS

The author is indebted to Dr. James Stallcop and Dr. Max Loewenstein for helpful criticism.

[9] See, e.g., M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions*, National Bureau of Standards Applied Mathematics Series (55) (U.S. Government Printing Office, Washington, D.C., 1964), p. 256.

[10] See, e.g., E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, Cambridge, England, 1927), p. 28.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

On the Combinatorial Structure of State Vectors in $U(n)$.* II. The Generalization of Hypergeometric Functions on $U(n)$ States

MIKAEL CIFTAN†
Department of Physics, Duke University, Durham, North Carolina

(Received 10 April 1968)

The derivation of the explicit algebraic expressions of the $SU(n)$ state vectors in the boson-operator realization is shown to lead to a generalization of hypergeometric functions. The $SU(3)$ state vectors are rederived by the combinatorial method—propounded in Paper I [J. Math. Phys. **10**, 221 (1969)] of this series of papers—and are shown to be represented by a hypergeometric distribution function and an associated generalization of the Young tableaux calculus. The $SU(4)$ state vectors are also derived to demonstrate the main features of the general $U(n)$ state vectors. The $SU(4)$ state vectors are expressed in terms of the constituents of Radon transforms.

1. INTRODUCTION

In Paper I of this series[1] it was shown that the boson-operator realization of the maximal and semimaximal state vectors of the irreducible representations of $U(n)$ are built upon combinatorial structure. First, the *lattice*[2] (the partially ordered set in the mathematical sense) of the invariants of $U(n)$ in the canonical chain $U(n) \supset U(n-1) \cdots \supset U(1)$ displays most explicitly the combinatorial[3] structure upon which the algebra of the state vectors is based; second, it was found that for these states the combinatorial calculations were implemented by a generalization of the Nakayama concept of a *hook*.

The present article starts, in Sec. 2, with a rederivation of the $SU(3)$ state vectors by the propounded combinatorial procedure; the details of the procedure are important in demonstrating why and how the ${}_2F_1$ hypergeometric function arises in $SU(3)$ from the combinatorial probabilistic hypergeometric distribution function—as a result of the associated generalized hook calculus. It is then shown that the associated combinatorial problem leads to a generalization of Young tableaux calculus, namely, a calculus over generalized *skew* diagrams.

In Sec. 3, it is demonstrated that a large class of the general $U(n)$ state vectors, when expressed in the boson-operator realization, can be expressed in closed form if we introduce a new combinatorial generalization of hypergeometric functions. It is interesting to note that this is the first time that such a generalization appears necessarily in a concrete mathematical context, namely group theory, rather than as an arbitrary generalization of the ${}_2F_1$ function to those of many variables.[4] It is this connection to group theory and Lie algebra[5] that makes the appearance of such functions rather interesting for both mathematics and physics; it is also in this context that the combinatorial procedures which offers a practical computational means (aside from elucidating structural content) becomes extremely valuable.

In our effort to uncover the complete structural content of all $U(n)$ states, we show in Sec. 4 that the *general* $SU(4)$ state vector expressed in terms of these generalized functions can be cast into the constituents of Radon transforms. In Paper I we saw that the $SU(4)$ group is sufficiently more general than $SU(2)$ and $SU(3)$ groups to reveal certain peculiarities of $SU(n)$. Here again we demonstrate such a peculiarity: the most general $SU(4)$ state, in closed form, is not a complete Radon transform but is expressed over the *constituents* of Radon transforms, a "folded" function, as we shall see, which seems to bear some relationship to the group geometry. It is hoped that the combinatorial method may shed some light on the possible existence of an even more general function in terms of which all $U(n)$ states could be expressed.

2. GENERAL SU_3 STATES

Next we want to give the details of the method of obtaining the *general* U_3 or SU_3 states by the use of the lowering operator E_{21} as was done by Baird and Biedenharn.[6] These details are important in demonstrating that the propounded combinatorial method admits of generalization.

* Supported in part by the Army Research Office (Durham) and the National Science Foundation.

† Present address: Department of Physics, Indiana University, Bloomington, Indiana.

[1] M. Ciftan and L. C. Biedenharn, J. Math. Phys. **10**, 221 (1969).

[2] Which makes the Weyl branching law (see Paper I) immediately transparent.

[3] In the sense of Gian-Carlo Rota, reference in Paper I.

[4] See the works of P. Appell, referred to in Ref. 9 below.

[5] See, for example, W. Miller, Jr., "Lie Algebras and Some Special Functions of Mathematical Physics," *Memoirs of the American Mathematical Society, Number 50* (American Mathematical Society, Providence, Rhode Island, 1964); W. Miller, Jr., *Lie Theory and Special Functions* (Academic Press Inc., New York, 1968); J. D. Talman, *Special Functions, A Group Theoretical Approach* (W. A. Benjamin, Inc., New York, 1968).

[6] G. E. Baird and L. C. Biedenharn, J. Math. Phys. **4**, 1449 (1963).

Consider the semimaximal (let "s.m." denote "semimaximal" and "max" denote "maximal" when used as subscripts of normalization constants) state of SU_3 on which we want to operate with $(E_{21})^{m_{12}-m_{11}}$. Thus,

$$V \equiv (E_{21})^{m_{12}-m_{11}} \left| \begin{pmatrix} m_{13} & & m_{23} & & 0 \\ & m_{12} & & m_{22} & \\ & & m_{12} & & \end{pmatrix} \right\rangle$$

$$= M_{\text{s.m.}}^{-\frac{1}{2}} (E_{21})^{m_{12}-m_{11}} \times (a_{12})^{m_{22}} (a_{13})^{m_{23}-m_{22}} \times (a_1)^{m_{12}-m_{23}} (a_3)^{m_{13}-m_{12}} |0\rangle$$

$$= M_{\text{s.m.}}^{-\frac{1}{2}} (a_{12})^{m_{22}} (a_3)^{m_{13}-m_{12}} (E_{21})^{m_{12}-m_{11}} \times (a_{13})^{m_{23}-m_{22}} (a_1)^{m_{12}-m_{23}} |0\rangle \tag{2.1}$$

(letting $n \equiv m_{12} - m_{11}$, $\alpha \equiv m_{23} - m_{22}$, $\beta \equiv m_{12} - m_{23}$),

$$= M_{\text{s.m.}}^{-\frac{1}{2}} (a_{12})^{m_{22}} (a_3)^{m_{13}-m_{12}} \times \sum_{k=0}^{n} \binom{n}{k} \frac{\alpha!}{(\alpha-k)!} (a_{13})^{\alpha-k} (a_{23})^k (E_{21})^{n-k} (a_1)^{\beta} |0\rangle$$

$$= M^{-\frac{1}{2}} (a_{12})^{m_{22}} (a_3)^{m_{13}-m_{12}} \times \sum_{k=0}^{n} \binom{n}{k} \frac{\alpha!}{(\alpha-k)!} \frac{\beta!}{(\beta-(n-k))!} \times (a_{13})^{\alpha-k} (a_{23})^k (a_1)^{\beta-(n-k)} (a_2)^{n-k} |0\rangle, \tag{2.2}$$

but

$$h_{\alpha,\beta}(k;n) \equiv \frac{\binom{\alpha}{k}\binom{\beta}{n-k}}{\binom{\alpha+\beta}{n}} = \binom{n}{k} \frac{\alpha!}{(\alpha-k)!} \frac{\beta!}{(\beta-n+k)!} \frac{(\alpha+\beta-n)!}{(\alpha+\beta)!}. \tag{2.3}$$

Therefore,

$$V = M_{\text{s.m.}}^{-\frac{1}{2}} (a_{12})^{m_{22}} (a_3)^{m_{13}-m_{12}} \times \frac{(\alpha+\beta)!}{(\alpha+\beta-n)!} \times (a_{13})^{\alpha} (a_1)^{\beta-n} (a_2)^n \times \sum_{k=0}^{n} h_{\alpha,\beta}(k;n) \left(\frac{a_{23}a_1}{a_{13}a_2}\right)^k |0\rangle. \tag{2.4}$$

But

$$\sum_{k=0}^{n} h_{\alpha,\beta}(k;n) \left(\frac{a_{13}a_1}{a_{13}a_2}\right)^k = A\ {}_2F_1(-n, -\alpha; \beta - n + 1; u), \tag{2.5}$$

where

$$A \equiv \frac{\beta!\,(\alpha+\beta-n)!}{(\beta-n)!\,(\alpha+\beta)!}, \quad u \equiv \frac{a_{13}a_1}{a_{13}a_2}, \tag{2.6}$$

and ${}_2F_1$ is a "hypergeometric function"; there exists a well-defined combinatorial meaning associated with Eq. (2.6), which we shall give in the sequel.

It will be shown that the coefficients $h_{\alpha,\beta}$ are already appropriately "normalized" in a combinatorial sense; therefore, Eq. (2.6) indicates that the square of the correct normalization constant, or rather the probability coefficient of the general U_3 states, is

$$\frac{1}{M_{\text{s.m. } U_3}} \times h_{\ldots}(x; \cdots) \times \binom{(m_{12}-m_{23})}{(m_{11}-m_{23})}, \tag{2.7}$$

the last binomial factor being necessary to effect the hook changes in the indicated section $(m_{12} - m_{33})$ after the m_{11} boundary is moved; it is, in fact, the square of the normalization constant of this $(E_{21})^{m_{12}-m_{11}}$ lowering operator. To show that

$$P_{\substack{\text{general} \\ SU_3}} = \frac{1}{M_{\text{s.m.}}} \times h_{\ldots}(x; s) \times \binom{(m_{12}-m_{23})}{(m_{11}-m_{23})}, \tag{2.8}$$

we look at the leading term, which is the $x = 0$ term, of h giving A:

$$\frac{1}{M_{\text{s.m.}}} : \frac{(m_{12}-m_{22}+1)!}{(m_{12}+1)!\,m_{22}!} \times \frac{(m_{13}-m_{23}+1)!}{(m_{13}-m_{22}+1)!\,(m_{23}-m_{22})!} \times \frac{1}{(m_{12}-m_{23})!} \frac{1}{(m_{13}-m_{12})!}, \tag{2.9a}$$

$$A \text{ of } h_{\ldots} : \frac{(m_{11}-m_{22})!\,(m_{12}-m_{23})!}{(m_{11}-m_{23})!\,(m_{12}-m_{22})!}, \tag{2.9b}$$

$$\binom{(m_{12}-m_{23})}{(m_{11}-m_{23})} : \frac{(m_{12}-m_{23})!}{(m_{11}-m_{23})!\,(m_{12}-m_{11})!}, \tag{2.9c}$$

whence the product of these gives

$$P_{\substack{\text{general} \\ SU_3}} = \frac{(m_{11}-m_{22})!\,(m_{12}-m_{23})!}{(m_{11}-m_{23})!\,(m_{12}-m_{22})!} \times \frac{(m_{12}-m_{22}+1)!\,(m_{13}-m_{23}+1)!}{(m_{12}+1)!\,m_{12}!\,(m_{13}-m_{22}+1)!\,(m_{23}-m_{22})!} \times \frac{1}{(m_{11}-m_{23})!\,(m_{12}-m_{11})!\,(m_{13}-m_{12})!}; \tag{2.10}$$

or again we may choose to use the normalization constant[7]:

$$\mathcal{N}_T^{-1} = \left[\frac{(m_{11}-m_{22})!\,(m_{12}-m_{22}+1)!}{(m_{12}-m_{11})!\,(m_{13}-m_{12})!\,(m_{12}-m_{22})!\,(m_{13}-m_{22}+1)!} \times \frac{(m_{12}-m_{23})!\,(m_{12}-m_{33}+1)!\,(m_{22}-m_{33})!}{(m_{23}-m_{22})!\,(m_{13}-m_{23})!\,(m_{13}-m_{33}+1)!\,(m_{23}-m_{33})!} \right]^{\frac{1}{2}} \tag{2.11}$$

[7] J. G. Nagel and M. Moshinsky, J. Math. Phys. 6, 682 (1965).

of the "total" lowering operator

$$(E_{21})^{m_{12}-m_{11}}(E_{32})^{m_{23}-m_{22}}(L_3^1)^{m_{13}-m_{12}} \tag{2.12}$$

(with $n_1 \equiv m_{13} - m_{12}$, $n_2 \equiv m_{23} - m_{22}$, $n_3 \equiv m_{12} - m_{11}$, $\alpha \equiv m_{33}$, $\beta \equiv m_{23} - m_{33}$, $\gamma \equiv m_{13} - m_{23}$) in

$$\begin{aligned}
&(E_{21})^{n_3}(E_{32})^{n_2}(L_3^1)^{n_1}\frac{1}{M^{\frac{1}{2}}_{\max U_3}}(a_{123})^{\alpha}(a_{12})^{\beta}(a_1)^{\gamma}|0\rangle \\
&= \frac{1}{M^{\frac{1}{2}}_{\max U_3}} \times \frac{\beta!}{(\beta-n_2)!} \times \frac{\gamma!}{(\gamma-n_1)!} \\
&\quad \times \frac{(\gamma+\beta+1)!}{(\gamma+\beta+1-n_1)!} \times (a_{123})^{\alpha}(a_{12})^{\beta-n_2}(a_3)^{n_1} \\
&\quad \times (E_{21})^{n_3}(a_{13})^{n_2}(a_1)^{\gamma-n_1}|0\rangle \qquad (2.13a) \\
&= \frac{1}{M^{\frac{1}{2}}_{\max U_3}}\frac{\beta!}{(\beta-n_2)!}\frac{\gamma!}{(\gamma-n_1)!} \\
&\quad \times \frac{(\gamma+\beta+1)!}{(\gamma+\beta+1-n_1)!} \times (a_{123})^{\alpha}(a_{12})^{\beta-n_2}(a_3)^{n_1} \\
&\quad \times \frac{(\gamma+n_2-n_1)!}{(\gamma+n_2-n_1-n_3)!}(a_{13})^{\beta-n_2}(a_1)^{\gamma-n_1-n_3}(a_2)^{n_3} \\
&\quad \times \sum_{k=0}^{n_3} h_{n_2,\gamma-n_1}(k;n_3)\left(\frac{a_{23}a_1}{a_{13}a_2}\right)^k |0\rangle. \qquad (2.13b)
\end{aligned}$$

Factoring A out of the last factor $h\ldots$, the factor

$$\frac{(\gamma-n_1)!}{(\gamma-n_1-n_3)!}\frac{(\gamma+n_2-n_1-n_3)!}{(\gamma+n_2-n_1)!}$$

as in Eq. (2.6), we obtain

$$\begin{aligned}
\frac{1}{M^{\frac{1}{2}}_{\substack{\text{general}\\ U_3}}} &= \mathcal{N}_T^{-1}\frac{1}{M^{\frac{1}{2}}_{\max U_3}}\frac{\beta!}{(\beta-n_2)!}\frac{\gamma!}{(\gamma-n_1)!} \\
&\quad \times \frac{(\gamma+\beta+1)!}{(\gamma+\beta+1-n_1)!} \times \frac{(\gamma-n_1)!}{(\gamma-n_1-n_3)!} \qquad (2.14a) \\
&\equiv \mathcal{N}_T^{-1}\frac{1}{M^{\frac{1}{2}}_{\max U_3}}G. \qquad (2.14b)
\end{aligned}$$

Rewriting the contributions, we have

$$\begin{aligned}
\mathcal{N}_T^{-1} &= \left[\frac{(m_{11}-m_{22})!\,(m_{12}-m_{22}+1)!}{(m_{12}-m_{11})!\,(m_{13}-m_{12})!\,(m_{12}-m_{22})!\,(m_{13}-m_{22}+1)!}\right. \\
&\quad \left. \times \frac{(m_{12}-m_{23})!\,(m_{12}-m_{33}+1)!\,(m_{22}-m_{33})!}{(m_{23}-m_{22})!\,(m_{13}-m_{23})!\,(m_{13}-m_{33}+1)!\,(m_{23}-m_{33})!}\right]^{\frac{1}{2}}, \qquad (2.15a) \\
\frac{1}{M^{\frac{1}{2}}_{\max U_3}} &= \left[\frac{(m_{13}-m_{33}+2)!\,(m_{23}-m_{33}+1)!}{(m_{13}+2)!\,(m_{23}+1)!\,m_{33}!}\frac{(m_{13}-m_{23}+1)!}{(m_{13}-m_{33}+1)!\,(m_{23}-m_{33})!\,(m_{13}-m_{23})!}\right]^{\frac{1}{2}}, \\
G &= \frac{(m_{23}-m_{33})!}{(m_{22}-m_{33})!}\frac{(m_{13}-m_{23})!}{(m_{12}-m_{23})!}\frac{(m_{13}-m_{33}+1)!}{(m_{12}-m_{33}+1)!}\frac{(m_{12}-m_{23})!}{(m_{11}-m_{23})!}. \qquad (2.15b)
\end{aligned}$$

Their product is

$$\begin{aligned}
\frac{1}{M^{\frac{1}{2}}_{\substack{\text{general}\\ U_3}}} &= \left[\frac{(m_{11}-m_{22})!\,(m_{12}-m_{23})!}{(m_{11}-m_{23})!\,(m_{12}-m_{22})!}\frac{(m_{12}-m_{22}+1)!}{(m_{12}+1)!\,m_{22}!}\right. \\
&\quad \left. \times \frac{(m_{13}-m_{23}+1)!}{(m_{13}-m_{22}+1)!\,(m_{23}-m_{22})!\,(m_{13}-m_{12})!\,(m_{12}-m_{11})!\,(m_{11}-m_{23})!}\right]^{\frac{1}{2}}. \qquad (2.16)
\end{aligned}$$

So far we have seen the usefulness of the representative tableaux both in the determination of the explicit algebraic form of the operator part as well as their normalization constants of the states. We now show that the representative tableaux also embody a combinatorial interpretation even for the expression of the *general* U_3 states [Eqs. (2.24) and (2.25)].

To arrive at the proposed interpretation, we need the following preliminary observation. Taking the SU_3 case depicted in Fig. 1, when we move the m_{11} boundary from its $m_{11} = m_{12}$ position (for the semimaximal state) as indicated, inserting a boson operator a_2 in the single box now available according to the prescription of the

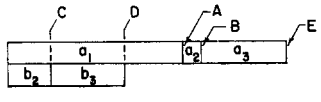


FIG. 1. The representative diagram corresponding to the $SU(3)$ state with $m_{12} - m_{11} = 1$, showing the origin of the hypergeometric function generated in the lowering procedure.

betweenness conditions, we are faced with the following dilemma: the hook of a box in the first row between boundaries C and D will have to pass over the a_2 boson to reach boundary E, yet the a_2 boson is not involved in the $a_{13} = (a_1 b_3 - a_3 b_1)$ entanglement! Therefore the hook, in this form, cannot be used due to the presence of the "foreign" boson a_2. If the hook

is not used, a powerful computational tool is lost! We shall see how one can resolve this dilemma below. This dilemma can be resolved when one recognizes that the associated *combinatorial* interpretation uses the hypergeometric distribution function which follows.

Consider a finite number of m balls, mp of which are white and $mq = m(1-p)$ of them black. When a sample of s balls are drawn out, one at a time (which will be eventually interpreted as moving the boundary of m_{11} one box at a time), *without replacements*, the chance of obtaining x white and $s-x$ black balls in s trials is

$$h_{mp,mq}(x,s) = \binom{mp}{x}\binom{mq}{s-x}\Big/\binom{m}{s} \tag{2.17}$$

$$= \frac{(mp)!}{x!\,(mp-x)!} \times \frac{(mq)!}{(s-x)!\,(mq-s+x)!} \times \frac{s!\,(m-s)!}{m!}$$

$$= A \times \frac{s!}{x!\,(s-x)!} \times \frac{(mp)!}{(mp-x)!} \times \frac{(mq-s)!}{(mq-s+x)!}, \tag{2.18}$$

where

$$A = \frac{mq!\,(m-s)!}{m!\,(mq-s)!}. \tag{2.19}$$

We then allow x to vary to account for the probability of obtaining all possible number of white balls among the s balls drawn, this being given by the coefficients of u^x in

$$A\left[1 + s\frac{mp}{mq-s+1} \times u + \frac{s(s-1)}{12} \times \frac{mp(mp-1)}{(mq-s+1)(mq-s+2)} \times u^2 + \cdots + \frac{mp(mp-1)\cdots(mp-s+1)}{(mq-s+1)(mq-s+2)\cdots mq} \times u^s\right]. \tag{2.20}$$

Relating this to our problem, as usual the properties endowed by the m objects (in our case ma's; see Fig. 2) is the entanglement property (the whiteness

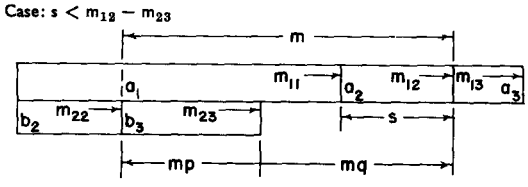


FIG. 2. The representative diagram of the $SU(3)$ general state for the case $s < m_{12} - m_{23}$.

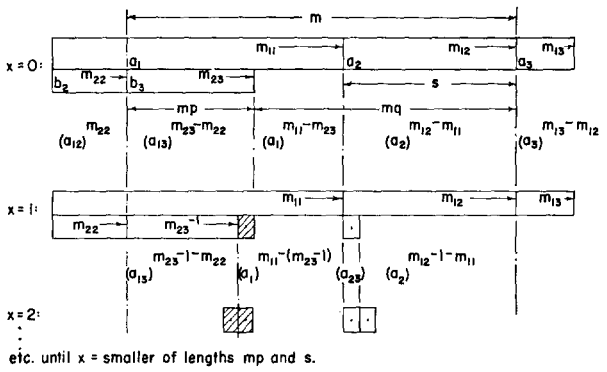


FIG. 3. The tableaux corresponding to the $x = 0, 1, \cdots$ terms of the general $SU(3)$ state vector when the hypergeometric function is expanded. U^x is interpreted as the necessary changes to be made to factor out a common factor:

$$(a_{12})^{m_{22}} \cdot (a_{13})^{m_{23}-m_{22}} \cdot (a_1)^{m_{11}-m_{23}} \cdot (a_2)^{m_{12}-m_{11}} \cdot (a_3)^{m_{13}-m_{22}}.$$

property $\equiv$ entanglement of a's with b_3's); mp of the a's, at the start, are entangled to b_3's and mq of the a's are nonentangled. s of the a's are drawn out (or put into the a_2 category), one at a time, without replacements, and we have derived the probability that, out of the a's that have been drawn out, there will be $1, 2, \cdots, s$ white (entangled to b_3) a's.

Diagrammatically, these correspond to the generalized tableaux[8] of Fig. 3. By making the substitutions

$$\begin{aligned} mq &\equiv m_{12} - m_{23}, \\ s &\equiv m_{12} - m_{11}, \\ mp &\equiv m_{23} - m_{22}, \end{aligned} \tag{2.21}$$

indicated by the diagrams, we obtain

$$\frac{(m_{11}-m_{22})!\,(m_{12}-m_{23})!}{(m_{11}-m_{23})!\,(m_{12}-m_{22})!} \times (a_1)^{m_{11}-m_{23}} \times (a_2)^{m_{12}-m_{11}} \times (a_3)^{m_{13}-m_{12}} \times {}_2F_1\left(m_{22}-m_{23}, m_{11}-m_{12}, m_{11}-m_{23}+1; \frac{a_1 a_{23}}{a_2 a_{13}}\right)|0\rangle. \tag{2.22}$$

To this we multiply the initial $M^{-\frac{1}{2}}_{\text{s.m.}\,SU_3}$ as well as the operator parts that were not affected and left out. Also, moving the m_{11} boundary to its general position has changed the hooks in the $(m_{12}-m_{23})$ portion; therefore these hooks need to be readjusted by the factor

$$\left[\frac{(m_{12}-m_{23})!}{(m_{12}-m_{11})!\,(m_{11}-m_{23})!}\right]^{\frac{1}{2}}. \tag{2.23}$$

Collecting all factors, we obtain the algebraic

[8] M. Ciftan and L. C. Biedenharn, Science **154**, 418 (1966).

expression of the general SU_3 state:

$$\left|\begin{bmatrix} m_{13} & & m_{23} & & 0 \\ & m_{12} & & m_{22} & \\ & & m_{11} & & \end{bmatrix}\right\rangle = N(a_{12})^{m_{22}}(a_{13})^{m_{23}-m_{22}} \times (a_1)^{m_{11}-m_{23}}(a_2)^{m_{12}-m_1}$$
$$\times (a_3)^{m_{13}-m_{12}} \times {}_2F_1\left(m_{22}-m_{23}, m_{11}-m_{12}, m_1-m_{23}+1; \frac{a_1a_{23}}{a_2a_{13}}\right)|0\rangle, \quad (2.24)$$

where

$$N^2 = \frac{(m_{11}-m_{22})!\,(m_{12}-m_{23})!}{(m_{11}-m_{23})!\,(m_{12}-m_{22})!} \times \frac{(m_{12}-m_{22}+1)!}{(m_{12}+1)!\,m_{22}!}$$
$$\times \frac{(m_{13}-m_{23}+1)!}{(m_{12}-m_{11})!\,(m_{11}-m_{23})!\,(m_{23}-m_{22})!\,(m_{13}-m_{22}+1)!\,(m_{13}-m_{12})!}. \quad (2.25)$$

We observe that, above, a particular choice (case: $m_{11} > m_{23}$) of the "general position" of the m_{11} boundary was made due to its simple tableaux, yet the final result was completely general. This we attribute to the "natural"-ness of the "coordinates" m_{ij} of the betweenness lattice. (We postpone the discussion of the more fundamental "lattice" and related "partial ordering" properties of these combinatorial structures to a future article.)

The result, Eq. (2.24), is the same as Eq. (44) of Baird and Biedenharn.[7]

3. A GENERALIZATION OF HYPERGEOMETRIC FUNCTIONS ON U_n STATES

To see how the $h_{\alpha,\beta}$ functions play a central role and generalize, as an example we perform

$$(E_{21})^n(a_1)^{\alpha_1}(a_{13})^{\alpha_2}(a_{14})^{\alpha_3}|0\rangle \equiv J \quad (3.1)$$

and obtain

$$J = \sum_{k_1=0}^{n}\sum_{k_2=0}^{n-k_1} \frac{(\alpha_1+\alpha_2+\alpha_3)!}{(\alpha_1+\alpha_2+\alpha_3-n)!} \times (a_1)^{\alpha_1}(a_{13})^{\alpha_2}(a_{14})^{\alpha_3-n}(a_{24})^n \times h_{\alpha_1,\alpha_2;N}(k_1,k_2;n) \times \left(\frac{a_2a_{14}}{a_1a_{24}}\right)^{k_1}\left(\frac{a_{23}a_{14}}{a_{13}a_{24}}\right)^{k_2}|0\rangle, \quad (3.2a)$$

where

$$h_{\alpha_1,\alpha_2;N}(k_1,k_2;n) \equiv \frac{\binom{\alpha_1}{k_1}\binom{\alpha_2}{k_2}\binom{N-\alpha_1-\alpha_2}{n-k_1-k_2}}{\binom{N}{n}}, \quad (3.3a)$$

$$N \equiv \alpha_1+\alpha_2+\alpha_3 \quad (3.3b)$$

is a generalization of Eq. (2.17); it has a clearly defined combinatorial interpretation similar to that of Eq. (2.17) but now with *three types* of balls, or in our problem *three* types of entanglement that we shall demonstrate below. To see that

$$\frac{(\alpha_1+\alpha_2+\alpha_3-n)!}{(\alpha_1+\alpha_2+\alpha_3)!} \times J \quad (3.2b)$$

in the form of Eq. (3.2a) defines a generalization of ordinary hypergeometric functions of Eq. (2.5) with two variables

$$\mu_1 \equiv \frac{a_2a_{14}}{a_1a_{24}}, \quad \mu_2 \equiv \frac{a_{13}a_{14}}{a_{23}a_{24}},$$

it is convenient to recast Eq. (3.3a) into the form

$$h_{\alpha_1,\alpha_2;N}(k_1,k_2;n) = \frac{\binom{\alpha_1}{k_1}\binom{N-\alpha_1}{n-k_1}}{\binom{N}{n}} \times \frac{\binom{\alpha_2}{k_2}\binom{(N-\alpha_1)-\alpha_2}{(n-k_1)-k_2}}{\binom{N-\alpha_1}{n-k_1}}$$
$$= h_{\alpha_1,(N-\alpha_1)}(k_1;n) \times h_{\alpha_2,N-\alpha_1-\alpha_2}(k_2;(n-k_1)) \quad (3.4a)$$

with

$$N \equiv \alpha_1+\alpha_2+\alpha_3, \quad (3.4b)$$

which shows that Eq. (3.2b) breaks up into the product over the constituents of two hypergeometric functions of the ${}_2F_1$ type. It is clear that with more *types* of antisymmetric forms [in Eq. (3.1)] on which the $(E_{ij})^n$ can operate without having a vanishing commutator, Eqs. (3.1) to (3.4) generalize to those of more variables.

We next show that

$$\sum_{k_1=0}^{n}\sum_{k_2=0}^{n-k_1} h_{\alpha_1,\alpha_2;N}(k_1,k_2;n)x_1^{k_1}x_2^{k_2}, \quad (3.5a)$$

which appears in Eq. (3.2), is proportional to Appell's F_1 function[9]

$$F_1(a;b_1,b_2;c;x_1,x_2) \equiv \sum\sum \frac{(a)_{k_1+k_2}(b_1)_{k_1}(b_2)_{k_2}}{k_1!\,k_2!\,(c)_{k_1+k_2}}x_1^{k_1}x_2^{k_2} \quad (3.6)$$

[9] W. N. Bailey, *Generalized Hypergeometric Series* (Cambridge University Press, London, 1935); L. J. Slater, *Generalized Hypergeometric Functions* (Cambridge University Press, Cambridge, 1966).

on two variables x_1 and x_2. Here, $(a)_k \equiv a(a+1)\times(a+2)\cdots(a+k-1)$, $(a)_0 \equiv 1$. This F_1 function is a particular generalization of the ${}_2F_1$ hypergeometric function

$$ {}_2F_1(a;b;c;x) = \sum_{k=0} \frac{(a)_k (b)_k}{k!\,(c)_k} x^k \qquad (2.5') $$

of Eq. (2.5). Letting

$$ a \equiv -n, $$
$$ b_1 \equiv -\alpha_1, $$
$$ b_2 \equiv -\alpha_2, $$
$$ c \equiv N - \sum \alpha_i - n + 1, $$

Eq. (3.6) becomes a *finite* series. Upon factoring

$$ (-1)^{\Sigma k_1} \times \prod_i (-1)^{k_i} = 1 \qquad (3.7) $$

after the substitution, we obtain the finite sum[10]

$$ F_1(-n; -\alpha_1, -\alpha_2; N - \sum \alpha_i - n + 1; x_1, x_2) $$
$$ = \sum_{k_1=0}^{n} \sum_{k_2=0}^{n-k_1} \left(\frac{n!}{(n - \sum k_i)!} \prod_{i=1}^{2} \frac{\alpha_i!}{(\alpha_i - k_i)!\, k_i!} \Big/ \frac{(N - \sum \alpha_i - n + \sum k_i)!}{(N - \sum \alpha_i - n)!} \right) x_1^{k_1} x_2^{k_2}. \qquad (3.8) $$

Next, to show that Eq. (3.5a) is essentially Eq. (3.8), we perform the rearrangement of terms in h:

$$ h_{\alpha_1,\alpha_2;N} $$
$$ = \frac{\alpha_1!}{(\alpha_1 - k_1)!\, k_1!} \frac{\alpha_2!}{(\alpha_2 - k_2)!\, k_2!} $$
$$ \times \frac{(N - \sum \alpha_i)!}{((N - \sum \alpha_i) - (n - \sum k_i))!\,(n - \sum k_i)!} $$
$$ \times \frac{(N-n)!\, n!}{N!} \frac{(N - \sum \alpha_i - n)!}{(N - \sum \alpha_i - n)!} \qquad (3.9a) $$
$$ = A_{\alpha_1,\alpha_2;N;n} \times \frac{n!}{(n - \sum k_i)!} \frac{\alpha_1!}{(\alpha_1 - k_1)!\, k!} \frac{\alpha_2}{(\alpha_2 - k_2)!\, k_2!} \Big/ \frac{(N - \sum \alpha_i - n + \sum k_i)!}{(N - \sum \alpha_i - n)!}, \qquad (3.9b) $$

where we have defined

$$ A_{\alpha_1,\alpha_2;N;n} \equiv \frac{(N - \sum \alpha_i)!\,(N-n)!}{(N - \sum \alpha_i - n)!\, N!}. \qquad (3.10) $$

Therefore, by Eq. (3.8),

$$ \sum_{k_1=0}^{n} \sum_{k_2=0}^{n-k_1} h_{\alpha_1,\alpha_2;N}(k_1, k_2; n) x_1^{k_1} x_2^{k_2} $$
$$ = A_{\alpha_1,\alpha_2;N;n} \times F_1(-n, -\alpha_1, \alpha_2; N - \sum \alpha_i - n + 1; x_1, x_2) \qquad (3.5b) $$

and, in general,

$$ \sum_{k_1=0}^{n} \sum_{k_2=0}^{n-k_1} \sum_{k_p=0}^{n-k_1-k_2\cdots-k_{p-1}} h_{\alpha_1,\cdots,\alpha_p;N}(k_1,\cdots,k_p;n) x_1^{k_1}\cdots x_p^{k_p} $$
$$ = A_{\alpha_1,\cdots,\alpha_p;N;n} F_1(-n, -\alpha_1, \cdots, -\alpha_p; N - \sum \alpha_i - n + 1; x_1, \cdots, x_p). \qquad (3.11) $$

Next we apply the same method of lowering operators to some SU_4 states to show how in actuality these generalized functions arise and to give the associated tableaux calculus. We want to demonstrate sufficient evidence that the argument might possibly be turned around, similar to the SU_3 case, such that, directly from the tableaux calculus, these $h\ldots$ functions (and, therefore, the explicit algebraic expressions of *any* state of any U_n) may be written down with relative ease.

Consider the SU_4 Gel'fand pattern and the maximal state for a given set of values of the representation labels m_{i4}, $i = 1, 2, 3$, $m_{44} = 0$. To obtain the expression of the general states, we can use the explicit expression of the semimaximal states of SU_4:

$$ |SU_4, \text{s.m.}\rangle = M_{\text{s.m.}}^{-\frac{1}{2}} (a_{123})^{m_{33}} (a_{124})^{m_{34}-m_{33}} (a_{12})^{m_{23}-m_{34}} \times (a_{14})^{m_{24}-m_{23}} (a_1)^{m_{13}-m_{24}} (a_4)^{m_{14}-m_{13}} |0\rangle, \qquad (3.12) $$

$M_{\text{s.m.}}^{-\frac{1}{2}}$ being evaluated as before, using the results of Paper I. Let

$$ \alpha_1 \equiv m_{33}, \qquad \alpha_4 \equiv m_{24} - m_{23}, $$
$$ \alpha_2 \equiv m_{34} - m_{33}, \qquad \alpha_5 \equiv m_{13} - m_{24}, $$
$$ \alpha_3 \equiv m_{23} - m_{34}, \qquad \alpha_6 \equiv m_{14} - m_{13}. $$

The general SU_4 state would then be obtained by

$$ |SU_4, \text{general}\rangle $$
$$ = \mathcal{N}^{-1} (L_2^1)^{m_{12}-m_{11}} (L_3^1)^{m_{13}-m_{12}} (L_3^2)^{m_{23}-m_{22}} |SU_4\rangle_{\text{s.m.}}, \qquad (3.13) $$

where $\mathcal{N}^{-1}$ is the lumped normalizing coefficient of the lowering operators. Observing the complexity which arises when L_3^1 is raised to a power, we abandon its use here (we postpone the discussion of this operation to the end of this paper) by restricting our consideration to SU_4 states with $m_{12} = m_{13}$. Letting

$$ n_1 \equiv m_{23} - m_{22}, $$
$$ n_2 \equiv m_{13} - m_{11} = m_{12} - m_{11};\ m_{13} = m_{12}, $$

and using Eq. (15) of Paper I repeatedly, we obtain

$$ K \equiv \left| \begin{pmatrix} m_{14} & & m_{24} & & m_{34} & & 0 \\ & m_{13} & & m_{23} & & m_{33} & \\ & & m_{13} & & m_{22} & & \\ & & & m_{11} & & & \end{pmatrix} \right\rangle $$
$$ = \mathcal{N}^{-1} \times M_{\text{s.m.}}^{-\frac{1}{2}} \times (E_{21})^{n_2} (E_{32})^{n_1} (a_{123})^{\alpha_1} (a_{124})^{\alpha_2} \times (a_{12})^{\alpha_3} (a_{14})^{\alpha_4} (a_1)^{\alpha_5} (a_4)^{\alpha_6} |0\rangle $$
$$ = N \times (E_{21})^{n_2} (a_{123})^{\alpha_1} (a_{14})^{\alpha_4} (a_1)^{\alpha_5} (a_4)^{\alpha_6} \times (E_{32})^{n_1} (a_{124})^{\alpha_2} (a_{12})^{\alpha_3} |0\rangle. \qquad (3.14a) $$

[10] The substitutions are $(a)_k \equiv a(a+1)\cdots(a+k-1)$, $(a)_k = (a-1+k)!/(a-1)!$, $n!/(n-k)! = n(n-1)(n-2)\cdots(n-k+1)$. Let $n = -a$. Then $n!/(n-k)! = (-a)(-a-1)(-a-2)\cdots(-a-k+1) = (-1)^k a(a+1)\cdots(a+k-1) = (-1)^k (a)_k$.

But, from Eqs. (2.5) and (2.6),

$$(E_{32})^{n_1}(a_{124})^{\alpha_2}(a_{12})^{\alpha_3}|0\rangle = \sum_{k_1=0}^{n_1}\binom{n_1}{k_1}\frac{\alpha_2!}{(\alpha_2-k_1)!}\frac{(\alpha_3)!}{(\alpha_3-n_1+k_1)!} \times (a_{124})^{\alpha_2-k_1}(a_{134})^{k_1}(a_{12})^{\alpha_3-n_1+k_1}(a_{13})^{n_1-k_1}|0\rangle \tag{3.15a}$$

$$= \frac{\alpha_3!}{(\alpha_3-n_1)!}(a_{124})^{\alpha_2}(a_{12})^{\alpha_3-n_1}(a_{13})^{n_1} \times {}_2F_1\left(-n_1, -\alpha_2, \alpha_3-n_1+1; \left(\frac{a_{134}a_{12}}{a_{124}a_{13}}\right)\right)|0\rangle. \tag{3.15b}$$

Thus,

$$K = \mathcal{N}^{-1} \times M_{\text{s.m.}}^{-\frac{1}{2}} \times (a_{123})^{\alpha_1}(a_4)^{\alpha_6} \times \sum_{k=0}^{n}\binom{n}{k_1}\frac{\alpha_2!}{(\alpha_2-k_1)!}\frac{\alpha_3!}{(\alpha_3-n_1+k_1)!} \times (a_{124})^{\alpha_2-k_1}(a_{12})^{\alpha_3-n_1+k_1}(E_{21})^{n_2} \times (a_{14})^{\alpha_4}(a_1)^{\alpha_5}(a_{134})^{k_1}(a_{13})^{n_1-k_1}|0\rangle. \tag{3.14b}$$

Next, performing the $(E_{21})^{n_2}$ operation in Eq. (3.14a), we obtain (with $k_5 \equiv n_2 - k_2 - k_3 - k_4$)

$$(E_{21})^{n_2}(a_{14})^{\alpha_4}(a_1)^{\alpha_5}(a_{134})^{k_1}(a_{13})^{n_1-k_1}|0\rangle = \sum_{k_2=0}^{n_2}\sum_{k_3=0}^{n_2-k_2}\sum_{k_4=0}^{n_2-k_2-k_3}\frac{n_2!}{k_2!\,k_3!\,k_4!\,k!} \times \frac{\alpha_4!}{(\alpha_4-k_2)!}\frac{\alpha_5!}{(\alpha_5-k_3)!}\frac{k_1!}{(k_1-k_4)!}\frac{(n_1-k_1)!}{(n_1-k_1-k_5)!} \times (a_{14})^{\alpha_4-k_2}(a_{24})^{k_2}(a_1)^{\alpha_5-k_3}(a_2)^{k_3} \times (a_{134})^{k_1-k_4}(a_{234})^{k_4}(a_{13})^{n_1-k_1-k_5}|0\rangle. \tag{3.16}$$

Combining Eqs. (3.14b) and (3.16), we have

$$K = \mathcal{N}^{-1} \times M_{\text{s.m.}}^{-\frac{1}{2}} \times \frac{(\alpha_2+\alpha_3)!}{(\alpha_2+\alpha_3-n_1)!} \times \frac{(\alpha_4+\alpha_5+n_1)!}{(\alpha_4+\alpha_5+n_1-n_2)!}(a_{123})^{\alpha_1}(a_4)^{\alpha_6}(a_{124})^{\alpha_2} \times (a_{12})^{\alpha_3-n_1}(a_{14})^{\alpha_4}(a_1)^{\alpha_5}(a_{13})^{n_1} \times \sum_{k_1=0}^{n_1}\sum_{k_2=0}^{n_2}\sum_{k_3=0}^{n_2-k_2}\sum_{k_4=0}^{n_2-k_2-k_3} h_{\alpha_2,\alpha_3}(k_1; n_1) \times h_{\alpha_4,\alpha_5,k_1,(n_1-k_1)}(k_2, k_3, k_4; n_2) \times \left(\frac{a_{12}}{a_{13}}\frac{a_{134}}{a_{124}}\right)^{k_1}\left(\frac{a_{24}}{a_{14}}\right)^{k_2}\left(\frac{a_2}{a_1}\right)^{k_3}\left(\frac{a_{234}}{a_{134}}\right)^{k_4}\left(\frac{a_{23}}{a_{13}}\right)^{k_5}|0\rangle, \tag{3.14c}$$

where

$$h_{\alpha_2,\alpha_3}(k_1; n_1) \equiv \binom{\alpha_2}{k_1}\binom{\alpha_3}{n_1-k_1}\Big/\binom{\alpha_2+\alpha_3}{n}, \tag{3.17}$$

$$h_{\alpha_4,\alpha_5,k_1,(n_1-k_1)}(k_2, k_3, k_4; n_2) \equiv \binom{\alpha_4}{k_2}\binom{\alpha_5}{k_3}\binom{k_1}{k_4}\binom{n_1-k_1}{n_2-k_2-k_3-k_4}\Big/\binom{\alpha_4+\alpha_5+n_1}{n_2}. \tag{3.18}$$

We next show the tableaux calculus associated with Eq. (3.16).

Consider the effect of $(E_{21})^n$ operator in Eq. (3.15a), shown in Fig. 4(a), starting with the tableaux of the semimaximal case; the m_{22} boundary is to be moved into general position, between m_{22} and m_{23} in accordance with the betweenness condition. As in SU_3, we move the m_{22} boundary with $m_{22} > m_{34}$ for convenience without losing generality of the derived expressions. The resulting changes in the expressions of the involved antisymmetric forms can be read off directly from the diagram, together with the numerical coefficients from the h functions involved. *Next*, we want to bring the m_{11} variable in the Gel'fand pattern to its general value from the $m_{11} = m_{12}$ value. The algebraic effect of this operation is given by Eq. (3.16), which again can be read off from the associated diagram, the part of Fig. 4(a) being involved is enlarged and depicted in Fig. 4(b). A study of these diagrams indicates that the whole expression (3.14c) for the SU_4 states with $m_{13} = m_{12}$ could have been read off these tableaux with the aid of the h function. The generalized hypergeometric functions associated with the $L_{t+1}^t = E_{t+1;t}$ (refer to the Gel'fand pattern) are of the form

$$\sum_{k_1=0}^{n}\sum_{k_2=0}^{n-k_1}\cdots\sum_{k_p=0}^{n-\Sigma k_1} h_{\alpha_1,\alpha_2,\cdots,\alpha_p;N} \times (k_1, k_2, \cdots, k_p; n)(u_1)^{k_1}\cdots(u_p)^{k_p} \tag{3.19}$$

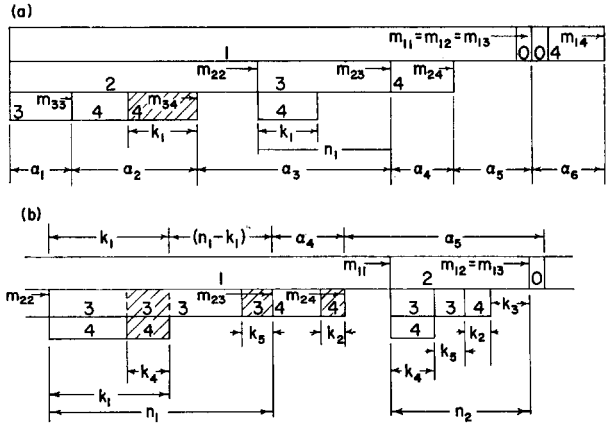


FIG. 4. The tableaux representing the algebraic operations that give the general $SU(4)$ states with $m_{12} = m_{13}$, indicating that the expression for these states can be read off directly from these tableaux in terms of generalized hypergeometric functions presented.

with the coefficients

$$h_{\alpha_1,\alpha_2,\cdots,\alpha_p;N}(k_1, k_2, \cdots, k_p; n)$$

$$= \binom{\alpha_1}{k_1}\binom{\alpha_2}{k_2}\cdots\binom{\alpha_p}{k_p}\binom{N-\sum_{i=1}\alpha_i}{n-\sum_{i=1}k_i}\Big/\binom{N}{n} \quad (3.20a)$$

$$= A_{\alpha_1,\alpha_2,\cdots,\alpha_p;N;n} \times \frac{n!}{(n-\sum k_i)} \times \prod_i \frac{\alpha_i!}{(\alpha_i-k_i)!\,k_i!}\frac{(N-\sum\alpha_i-n)!}{(N-\sum\alpha_i-(n-\sum k_i))!}, \quad (3.20b)$$

where

$$A_{\alpha_1,\alpha_2,\cdots,\alpha_p;N;n} \equiv \frac{(N-\sum\alpha_i)!}{(N-\sum\alpha_i-n)!}\frac{(N-n)!}{N!}. \quad (3.21)$$

Each such $(E_{i+1,i})^{n_i}$ operator contributes to the probability coefficient P of the state coefficients of the type

$$h_{\alpha_1,\cdots,\alpha_p;N}(k,\cdots,k_p;n_l) \times \binom{N-\sum\alpha_i}{n_l}. \quad (3.22)$$

The tableaux of Figs. 4(a) and 4(b) could themselves have been drawn with the aid of the betweenness condition alone. Thus the whole algebraic expression of these SU_4 states can be written down with the aid of a tableaux calculus. There remains the problem of removing the $m_{13} = m_{12}$ restriction or its equivalent in other U_n states.

We want to demonstrate that the *integral representations* of these hypergeometric functions show a connection with the structure of the representations of U_n; the fractional linear transformation of a variable t in these functions relate to raising and lowering operations as indicated by the following examples.

Consider the probability coefficient

$$h_{\alpha;\alpha+\beta}(k_1;n) \equiv \binom{\alpha}{k_1}\binom{\beta}{n-k_1}\Big/\binom{\alpha+\beta}{n} \quad (3.23a)$$

and its two expressions, using $k_1 + k_2 = n$,

$$h_{\alpha;\alpha+\beta}(k_1;n) = \frac{(\alpha+\beta-n)!}{(\alpha+\beta)!}\frac{\alpha!}{(\alpha-n)!}\frac{(-\beta)_{k_2}(-n)_{k_2}}{k_2!\,(\alpha-n+1)_{k_2}} \quad (3.23b)$$

$$= \frac{(\alpha+\beta-n)!}{(\alpha+\beta)!}\frac{\beta!}{(\beta-n)!}\frac{(-\alpha)_{k_1}(-n)_{k_1}}{k_1!\,(\beta-n+1)_{k_1}}, \quad (3.23c)$$

whence

$$(E_{21})^n(a_{13})^\alpha(a_1)^\beta|0\rangle = \frac{\beta!}{(\beta-n)!}(a_{13})^\alpha(a_1)^{\beta-n}(a_2)^n \times \sum_{k_1=0}^{n}\frac{(-\alpha)_{k_1}(-n)_{k_1}}{k_1!\,(\beta-n+1)_{k_1}}\left(\frac{a_{23}a_1}{a_{13}a_2}\right)^{k_1}|0\rangle \quad (3.24a)$$

$$= \frac{\alpha!}{(\alpha-n)!}(a_{13})^{\alpha-n}(a_1)^\beta(a_{23})^n \times \sum_{k_2=0}^{n}\frac{(-\beta)_{k_2}(-n)_{k_2}}{k_2!\,(\alpha-n+1)_{k_2}}\left(\frac{a_{13}a_2}{a_{23}a_1}\right)^{k_2}|0\rangle, \quad (3.24b)$$

which will be shown to be related to the transformation $z \to z^{-1}$ of ${}_2F_1$:

$${}_2F_1(a,b;c;z) = \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)}(-z)^{-a} \times {}_2F_1(a,1-c+a;1-b+a;z^{-1}) + \frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)}(-z)^{-b} \times {}_2F_1(b,1-c+b;1-a+b;z^{-1}). \quad (3.25)$$

Rewriting the above, we have

$$\sum_{k_2=0}^{n}\frac{(-\beta)_{k_2}(-n)_{k_2}}{k_2!\,(\alpha-n+1)_{k_2}}\left(\frac{a_{13}a_2}{a_{23}a_1}\right)^{k_2}|0\rangle = \frac{(\alpha-n)!}{\alpha!}\frac{\beta!}{(\beta-n)!}\left(\frac{a_{13}a_2}{a_{23}a_1}\right)^n \times \sum_{k_1=0}^{n}\frac{(-\alpha)_{k_1}(-n)_{k_1}}{k_1!\,(\beta-n+1)_{k_1}}\left(\frac{a_{23}a_1}{a_{13}a_2}\right)^{k_1}|0\rangle. \quad (3.26)$$

Identifying $-\beta \equiv a$, $-n \equiv b$, $\alpha - n + 1 \equiv c$, $z \equiv a_{13}a_2/a_{23}a_1$, we have

$$\frac{(\alpha-n)!}{\alpha!}\frac{\beta!}{(\beta-n)!} \doteq \frac{\Gamma(c)}{\Gamma(c-b)}\frac{\Gamma(a-b)}{\Gamma(a)}.$$

We obtain the left-hand side of Eq. (3.25) and *only the second term* of the right-hand side; the first term on the right-hand side vanishes for this identification. The vanishing of the first term is a curious phenomenon (in this context) and it appears not only in the *transformation of the variable z* but also in the use of contiguous relations *in the boson-operator* realization.

One can also examine the expression

$$(E_{21})^n(a_{13})^\alpha(a_1)^\beta|0\rangle = \frac{\beta!}{\beta-n}(a_{13})^\alpha(a_1)^{\beta-n}(a_2)^n \times \sum_{k_1=0}^{n}\frac{(-\alpha)_{k_1}(-n)_{k_1}}{k_1!\,(\beta-n+1)_{k_1}}\left(\frac{a_{23}a_1}{a_{13}a_2}\right)^{k_1}|0\rangle \quad (3.27)$$

and the expression, with $k_1 + k_2 = n$,

$$(E_{21})^n(a_{13})^\alpha(a_1)^\beta|0\rangle = \frac{\alpha!}{(\alpha-n)!}(a_{13})^{\alpha-n}(a_1)^{\beta-n}(a_{12}a_3)^n \times \sum_{k_2=0}^{n}\frac{(\alpha+\beta-n+1)_{k_2}(-n)_{k_2}}{k_2!\,(\alpha-n+1)_{k_2}}\left(\frac{a_{13}a_2}{a_{12}a_3}\right)^{k_2}|0\rangle \tag{3.28}$$

obtained by using the vanishing determinant

$$a^{112}_{123} = 0 \Rightarrow a_1a_{23} = a_2a_{13} - a_3a_{12} \tag{3.29}$$

demonstrating the transformation

$$z \to \frac{1}{1-z}, \quad z \equiv \frac{a_{23}a_1}{a_{13}a_2}, \quad \frac{1}{1-z} = \frac{a_{13}a_2}{a_{12}a_3}. \tag{3.30}$$

Again there exists the transformation of the ${}_2F_1$ functions

$$\begin{aligned}{}_2F_1(a,b;c;z) &= (1-z)^{-a}\frac{\Gamma(c)\Gamma(b-a)}{\Gamma(c-a)\Gamma(b)} \times {}_2F_1\left(a, c-b; 1+a-b; \frac{1}{1-z}\right) \\ &\quad + (1-z)^{-b}\frac{\Gamma(c)\Gamma(a-b)}{\Gamma(c-b)\Gamma(a)} \times {}_2F_1\left(c-a, b; 1-z+b; \frac{1}{1-z}\right).\end{aligned} \tag{3.31}$$

Thus

$$\sum_{k_1=0}^{n}\frac{(-\alpha)_{k_1}(-n)_{k_1}}{k_1!\,(\beta-n+1)_{k_1}}\left(\frac{a_{23}a_1}{a_{13}a_2}\right)^{k_1}|0\rangle = \frac{\alpha!}{(\alpha-n)!}\frac{(\beta-n)!}{\beta!}\left(\frac{a_{12}a_3}{a_{13}a_2}\right)^n \times \sum_{k_2=0}^{n}\frac{(\alpha+\beta-n+1)_{k_2}(-n)_{k_2}}{k_2!\,(\alpha-n+1)_{k_2}}\left(\frac{a_{13}a_2}{a_{12}a_3}\right)^{k_2}|0\rangle. \tag{3.32}$$

Identifying

$$a = -\alpha, \quad b = -n, \quad c = \beta - n + 1,$$

we obtain

$$\frac{\alpha!}{(\alpha-n)!}\frac{(\beta-n)!}{\beta!} \doteq \frac{\Gamma(a-b)}{\Gamma(a)}\frac{\Gamma(c)}{\Gamma(c-b)}, \tag{3.33}$$

again giving the second term of the right-hand side of Eq. (3.31), but not the first term of the same!

Although Fig. 4(b) does not lend itself to a tableau calculus (at this point), its transformed form [Fig. 4(a)] does. This example indicates that vanishing determinantal identities may be used with the proviso that the resulting expression be transformed to a combinatorially meaningful form if the appropriate transformation laws are known and if such a combinatorially meaningful result is desired.

These examples demonstrate that the boson-operator realization itself has a deeper connection with the integral representation of these functions; furthermore, the boson-operator realization is a special *sub*structure of the structure of these functions since only special terms appear in the transformation of the arguments of ${}_2F_1$. The same observation is made with respect to the contiguous relation identities wherein the vanishing determinants give restricted relations.

In view of the importance of integral representations of these functions, we want to carry this analysis one step further at this time. We next want to show that these generalized ${}_2F_1$ functions (i.e., those of many variables) encountered above are in fact the Radon transform[11] of a product of linear forms.

Let the symbol V denote the Radon transform $\overset{\mathrm{V}}{f}(\xi, p)$,

$$\overset{\mathrm{V}}{f}(\xi, p) \equiv \int f(x)\delta(p - (\xi, x))\,dx, \tag{3.34}$$

of the function $f(x)$, where

$$x \equiv (x_1, x_2, \cdots, x_n), \quad dx = dx_1 \cdot dx_2 \cdots dx_n,$$

with

$$(\xi, x) = \xi_1x_1 + \xi_2x_2 + \cdots + \xi_nx_n = p$$

denoting a hyperplane in the oriented n-demensional real affine space. The ordinary hypergeometric function

$${}_2F_1(\alpha,\beta,\gamma;t) = \frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma-\beta)} \times \int_0^1 x_1^{\beta-1}(1-x_1)^{\gamma-\beta-1}(1-tx_1)^{-\alpha}\,dx_1 \tag{3.35a}$$

can be cast into the ratio of two Radon transforms,

$${}_2F_1(\alpha,\beta,\gamma;t) = \frac{[(\xi_0^{(1)}, x)_+^{\beta-1}(\xi_0^{(2)}, x)_+^{\gamma-\beta-1}(\xi_0^{(3)}, x)_+^{-\alpha}]^{\mathrm{V}}}{[(\xi_0^{(1)}, x)_+^{\beta-1}(\xi_0^{(2)}, x)_+^{\gamma-\beta-1}]^{\mathrm{V}}}, \tag{3.35b}$$

as follows: the denominator above corresponds to the beta function in front of the integral, while the numerator to the latter. The + signs above indicate that

[11] I. M. Gel'fand, M. I. Graev, and N. Ya. Vilenkin, *Generalized Functions* (Academic Press Inc., New York, 1966), Vol. V.

integration is to be carried over the positive "octant" of the two-dimensional space that we shall now find.

Let $x_2 \equiv 1 - x_1$ in the integrand; then the integrand is

$$(x_1)^{\beta-1}(x_2)^{\gamma-\beta-1}[(1-t)x_1 + x_2]^{-\alpha}$$

and the particular linear form which is the "hyperplane" $(\xi, x) = p$. The argument of the δ function in the Radon transform of this function becomes

$$x_1 + x_2 = 1.$$

Denoting

$$\xi_0^{(1)} \equiv (1, 0), \quad \xi_0^{(2)} \equiv (0, 1), \quad \xi_0^{(3)} \equiv ((1-t), 1),$$

the integral is cast into the particular Radon transform indicated by the numerator of the ${}_2F_1$ function in Eq. (3.35b). The coefficients in Eq. (3.35a) define the beta function

$$B(\beta, \gamma - \beta) \equiv \frac{\Gamma(\beta)\Gamma(\gamma-\beta)}{\Gamma(\gamma)}, \tag{3.36}$$

which is the special case $\alpha = 0$ of the integral in Eq. (3.35a) and therefore obviously corresponds to the denominator in Eq. (3.35b).

Next we want to show that Appell's generalization of ${}_2F_1$ functions, the F_1's that arise in the representations of U_n (as demonstrated above), are also Radon transforms of a product of linear forms.

Consider the integral representation (Ref. 8, p. 76) of the F_1 function on *two* variables,

$$F_1(\alpha; \beta, \beta'; \gamma; t_1, t_2) = \frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\beta')\Gamma(\gamma-\beta-\beta')} \times \iint x_1^{\beta-1}x_2^{\beta'-1}(1-x_1-x_2)^{\gamma-\beta-\beta'-1} \times (1 - t_1x_1 - t_2x_2)^{-\alpha}\, dx_1\, dx_2, \tag{3.37a}$$

taken over the triangle $x_1 \geq 0$, $x_2 \geq 0$, $x_1 + x_2 \leq 1$.

Let

$$x_3 \equiv 1 - x_1 - x_2,$$

which defines the hypersurface

$$(\xi, x) = p \to x_1 + x_2 + x_3 = 1, \quad x_i \geq 0.$$

This is the triangular area, the intersection of the hyperplane with the positive octant of 3-space, over which the integration contributes. Thus the integral is the Radon transform of the function

$$(x_1)_+^{\beta-1}(x_2)_+^{\beta'-1}(x_3)_+^{\gamma-\beta-\beta'-1} \times ((1-t_1)x_1 + (1-t_2)x_2 + x_3)_+^{-\alpha}.$$

Again the gamma functions in front of the integral in Eq. (3.37a) define the corresponding generalized beta function $B(\beta, \beta', \gamma - \beta - \beta')$, the Radon transform of the beta function being obtained from that of the integral by letting $\alpha = 0$. Thus we have

$$F_1(\alpha; \beta, \beta', \gamma; t_1, t_2) = \frac{[(\xi_0^{(1)}, x)_+^{\beta-1}(\xi_0^{(2)}, x)_+^{\beta'-1}(\xi_0^{(3)}, x)_+^{\gamma-\beta-\beta'-1}(\xi_0^{(4)}, x)_+^{-\alpha}]^\nabla}{[(\xi_0^{(1)}, x)_+^{\beta-1}(\xi_0^{(2)}, x)_+^{\beta'-1}(\xi_0^{(3)}, x)_+^{\gamma-\beta-\beta'}]^\nabla}, \tag{3.37b}$$

where

$$\xi_0^{(1)} \equiv (1, 0, 0),$$
$$\xi_0^{(2)} \equiv (0, 1, 0),$$
$$\xi_0^{(3)} \equiv (0, 0, 1),$$
$$\xi_0^{(4)} \equiv ((1-t_1), (1-t_2), 1),$$
$$\xi_0 \equiv (1, 1, 1), \quad p = 1 \quad \text{in} \quad (\xi_0, x) = p,$$

the triangular plane.

It is hoped that these connections will provide further clues as to the possible closed form of the explicit algebraic expressions of the general U_n states in terms of the boson-operator calculus.

Using the Radon form of the ${}_2F_1$ function, we can rewrite the general SU_3 states with its probability coefficient (the *square* of the normalization constant N^{-1} states) as

$$N^{-1}\,|SU_3\rangle = \frac{1}{M_{\text{s.m. } SU_3}} \binom{m_{12} - m_{23}}{m_{11} - m_{23}}\, {}_2A_1 \times (a_{12})^{m_{22}}(a_3)^{m_{13}-m_{12}}(a_{13})^{m_{23}-m_{22}}(a_1)^{m_{11}-m_{23}}(a_2)^{m_{12}+m_{11}} \times \frac{[(\xi_0^{(1)}, x)^{m_{12}-m_{23}-1}(\xi_0^{(2)}, x)^{m_{12}-m_{22}}(\xi_0^{(3)}, x)^{m_{11}-m_{12}+1}]^\nabla}{[(\xi_0^{(1)}, x)^{m_{12}-m_{23}-1}(\xi_0^{(2)}, x)^{m_{12}-m_{22}}]^\nabla}, \tag{3.38}$$

where

$${}_2A_1 \equiv \frac{(m_{12}-m_{23})!\,(m_{11}-m_{22})!}{(m_{11}-m_{23}+1)!\,(m_{12}-m_{22})!},$$
$$\xi_0^{(1)} \equiv (1, 0), \quad \xi_0^{(2)} \equiv (0, 1),$$
$$\xi_0^{(3)} \equiv \left(\frac{a_3a_{12}}{a_2a_{13}}, 1\right) = (1-t, 1),$$
$$t \equiv \frac{a_1a_{23}}{a_2a_{13}}.$$

4. THE GENERAL SU_4 STATES

In the previous sections the L_3^1 operator was neglected in calculating the SU_4 states, thereby deriving only special cases of the general SU_4 states. We now show that, starting with the semimaximal SU_4 states, one can apply the $(L_3^1)^n$ operator and indeed obtain a closed form (see Fig. 5).

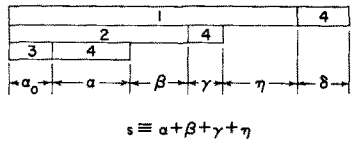


FIG. 5. The simplified diagram representing the $SU(4)$ semimaximal states.

We need to find

$$\left|\begin{matrix}\text{general}\\ SU_4\end{matrix}\right\rangle = \mathcal{N}^{-1}_{(E_{21})^{n_3}}\mathcal{N}^{-1}_{(E_{32})^{n_2}}\mathcal{N}^{-1}_{(L_3^1)^{n_1}}M^{-\frac{1}{2}}_{\text{s.m. }SU_4} \times (E_{21})^{n_3}(E_{32})^{n_2}(L_3^1)^{n_1} \times (a_{123})^{\alpha_0}(a_{124})^{\alpha}(a_{12})^{\beta}(a_{14})^{\gamma}(a_1)^{\eta}(a_4)^{\delta}\,|0\rangle. \tag{4.1}$$

We note that L_3^1 commutes with a_{123}, a_{34}, a_3, a_4. To start with, we find

$$\begin{aligned} &L_3^1(a_{124})^{\alpha}(a_{12})^{\beta}(a_{14})^{\gamma}(a_1)^{\eta}\,|0\rangle \\ &\quad = \eta(\alpha+\beta+\gamma+\eta+1) \times (a_{124})^{\alpha}(a_{12})^{\beta}(a_{14})^{\gamma}(a_1)^{\eta-1}a_3\,|0\rangle \\ &\qquad + \gamma(\alpha+\beta+\gamma+\eta+1) \times (a_{124})^{\alpha}(a_{12})^{\beta}(a_{14})^{\gamma-1}(a_1)^{\eta}a_{34}\,|0\rangle \\ &\qquad - \eta\alpha(a_{124})^{\alpha-1}(a_{12})^{\beta}(a_{14})^{\gamma}(a_1)^{\eta-1}a_{123}a_4\,|0\rangle \end{aligned} \tag{4.2}$$

and

$$\begin{aligned} I &\equiv (L_3^1)^{n_1}(a_{124})^{\alpha}(a_{12})^{\beta}(a_{14})^{\gamma}(a_1)^{\eta}\,|0\rangle \\ &= \sum_{k_1=0}^{n_1}\sum_{k_2=0}^{n_1-k_1}(-1)^{k_1}\frac{n_1!}{k_1!\,k_2!\,(n_1-k_1-k_2)!} \times \frac{\eta!}{(\eta-n_1+k_2)!}\frac{\gamma!}{(\gamma-k_2)!}\frac{\alpha!}{(\alpha-k_1)!} \\ &\quad \times (s-2-n_1)(s-2-n_1+1) \\ &\quad \times (s-2-n_1+2)\cdots(s-2-n_1+(n_1-k_1)-1) \\ &\quad \times (a_{124})^{\alpha-k_1}(a_{12})^{\beta}(a_{14})^{\gamma-k_2}(a_1)^{\eta-n_1+k_2} \\ &\quad \times (a_{123}a_4)^{k_1}(a_{34})^{k_2}(a_3)^{n_1-k_1-k_2}\,|0\rangle. \end{aligned} \tag{4.3a}$$

Noting that the product over the factors having s is

$$(s-2-n_1)_{n_1-k_1} = \frac{\Gamma(s-2)}{\Gamma(s-2-n_1)}\frac{(-1)^{k_1}}{(3-s)_{k_1}}, \tag{4.4}$$

where we have used

$$(a)_{-k} = \frac{\Gamma(a-k)}{\Gamma(a)} = \frac{(-1)^k}{(1-a)_k}, \tag{4.5}$$

we obtain

$$\begin{aligned} I &\equiv \frac{\Gamma(s-2)}{\Gamma(s-2-n_1)}\sum_{k_1}\sum_{k_2}\frac{(-n_1)_{k_1+k_2}(-\alpha)_{k_1}(-\gamma)_{k_2}}{k_1!\,k_2!\,(3-s)_{k_1}(\eta-n_1+1)_{k_2}} \times \left(\frac{a_4a_{123}}{a_3a_{124}}\right)^{k_1}\left(\frac{a_1a_{34}}{a_3a_{14}}\right)^{k_2}|0\rangle \qquad (4.3b) \\ &= \frac{\Gamma(s-2)}{\Gamma(s-2-n_1)}F_2\left(-n_1;\,-\alpha,\,-\gamma;\; 3-s,\,\eta-n_1+1;\,\frac{a_4a_{123}}{a_3a_{124}},\,\frac{a_1a_{34}}{a_3a_{14}}\right)|0\rangle. \qquad (4.3c) \end{aligned}$$

But

$$\begin{aligned} &F_2(\alpha;\beta,\beta';\gamma,\gamma';t_1,t_2) \\ &\quad = \frac{\Gamma(\gamma)\Gamma(\gamma')}{\Gamma(\beta)\Gamma(\beta')\Gamma(\gamma-\beta)\Gamma(\gamma'-\beta)} \times \int_0^1\int_0^1 x_1^{\beta-1}x_2^{\beta'-1}(1-x_1)^{\gamma-\beta-1}(1-x_2)^{\gamma'-\beta'-1} \\ &\qquad \times (1-t_1x_1-t_2x_2)^{-\alpha}\,dx_1\,dx_2 \end{aligned} \tag{4.6a}$$

over the triangle $x_1 \geq 0$, $x_2 \geq 0$, $x_1 + x_2 \leq 1$. Let $x_3 \equiv 1 - x_1 - x_2$ as before; the integral is then the Radon transform of

$$(x_1)_+^{\beta-1}(x_2)_+^{\beta'-1}(x_2+x_3)_+^{\gamma-\beta-1}(x_1+x_3)_+^{\gamma'-\beta'-1} \times ((1-t_1)x_1+(1-t_2)x_2+x_3)_+^{-\alpha}.$$

The gamma functions in front give the inverse of the product of two beta functions. Therefore,

$$F_2(\alpha;\beta,\beta';\gamma,\gamma';t_1,t_2) = \frac{[(\xi_0^{(1)},x)_+^{\beta-1}(\xi_0^{(2)},x)_+^{\beta'-1}(\xi_0^{(3)},x)_+^{\gamma-\beta-1}(\xi_0^{(4)},x)_+^{\gamma'-\beta'-1}(\xi_0^{(5)},x)_+^{-\alpha}]^{\nu}}{[(\xi_0^{(1)},x)_+^{\beta-1}(\xi_0^{(2)},x)_+^{\beta'-1}(\xi_0^{(3)},x)_+^{\gamma-\beta-1}(\xi_0^{(4)},x)_+^{\gamma'-\beta'-1}]^{\nu}}, \tag{4.6b}$$

where

$$\begin{aligned} \xi_0^{(1)} &\equiv (1,0,0), \\ \xi_0^{(2)} &\equiv (0,1,0), \\ \xi_0^{(3)} &\equiv (0,1,1), \\ \xi_0^{(4)} &\equiv (1,0,1), \\ \xi_0^{(5)} &\equiv (1-t_1,1-t_2,1). \end{aligned}$$

In fact all F_1, F_2, and F_3 type functions can be cast into Radon forms.

The other two lowering operators $(E_{32})^{n_2}$ and $(E_{21})^{n_3}$, when operating on the F_2 function above, produce, as before, an ${}_2F_1$ function and an F_1 function on three variables, respectively and in that order; we obtain

$$\begin{aligned} \left|\begin{matrix}\text{general}\\ SU_4\end{matrix}\right\rangle &= \mathcal{N}^{-1}_{(E_{21})^{n_3}}\mathcal{N}^{-1}_{(E_{32})^{n_2}}\mathcal{N}^{-1}_{(L_3^1)^{n_1}}M^{-\frac{1}{2}}_{\text{s.m. }SU_4}\frac{\eta!\,(\gamma+\eta-n_1+n_2)!}{(\eta-n_1)!\,(\gamma+\eta-n_1+n_2-n_3)!} \\ &\quad \times (a_{123})^{\alpha_0}(a_4)^{\delta}(a_{124})^{\alpha}(a_{12})^{\beta-n_2}(a_{14})^{\gamma}(a_1)^{\eta-n_1}(a_3)^{n_1}(a_{13})^{n_2-n_3}(a_{23})^{n_3} \\ &\quad \times \sum_{k_1=0}^{n_1}\sum_{k_2=0}^{n_1-k_1}\sum_{k_3=0}^{n_2}\sum_{k_4=0}^{n_3}\sum_{k_5=0}^{n_3-k_4}\sum_{k_6=0}^{n_3-k_4-k_5}(-1)^{k_1}\frac{(-n_1)_{k_1+k_2}(-\alpha)_{k_1}(-\gamma)_{k_2}}{k_1!\,k_2!\,(\eta-n_1+1)_k} \\ &\quad \times (s-2-n_1)_{n_1-k_1} \times \frac{(\alpha-k_1+\beta)!}{(\alpha-k_1+\beta-n_2)!}h_{(\alpha-k_1),\beta}(k_3;n_2) \\ &\quad \times h_{(\gamma-k_2),(\eta-n_1+k_2),k_3,(n_2-k_3)}(k_4,k_5,k_6;n_3) \\ &\quad \times \left(\frac{a_4a_{123}}{a_3a_{124}}\right)^{k_1}\left(\frac{a_1a_{34}}{a_3a_{14}}\right)^{k_2}\left(\frac{a_{12}a_{134}}{a_{13}a_{124}}\right)^{k_3}\left(\frac{a_{13}a_{24}}{a_{14}a_{23}}\right)^{k_4}\left(\frac{a_2a_{13}}{a_1a_{23}}\right)^{k_5}\left(\frac{a_{13}a_{234}}{a_{23}a_{134}}\right)^{k_6}|0\rangle, \end{aligned} \tag{4.6c}$$

where

$$s \equiv \alpha + \beta + \gamma + \eta.$$

Each h function above by itself gives a Radon transform. To see if this whole expression can be put into a "folded" single Radon form, we investigate the "semi-semimaximal" SU_4 states, i.e., the states with only $m_{12} = m_{11}$ and the rest of the m_{ik}'s in general position in the Gel'fand pattern. The relevant parts give the sum

$$\sum_{k_1}\sum_{k_2}\sum_{k_3}\frac{(-n_1)_{k_1+k_2}(-\gamma)_{k_2}(-n_2)_{k_3}(-\alpha)_{k_1+k_3}}{k_1!\,k_2!\,k_3!(3-s)_{k_1}(\eta-n_1+1)_{k_2}(\beta-n_2+1)_{k_3}} \times \left(\frac{a_4a_{123}}{a_3a_{124}}\right)^{k_1}\left(\frac{a_1a_{34}}{a_3a_{14}}\right)^{k_2}\left(\frac{a_{12}a_{134}}{a_{13}a_{124}}\right)^{k_3}. \quad (4.7a)$$

Casting this into general form and using the identity

$$(d)_{l+m} = (d+l)_m \cdot (d)_l, \quad (4.8)$$

we obtain

$$\sum_l\sum_m\sum_n \frac{(a)_{l+m}(b)_m(c)_n(d)_{l+n}}{(1)_l(1)_m(1)_n(e)_l(f)_m(g)_n}\,x^l y^m z^n = \sum_l\sum_m \frac{(a)_{l+m}(b)_m(d)_l}{(1)_l(1)_m(e)_l(f)_m}\,x^l y^m \sum_n \frac{(c)_n(d+l)_n}{(1)_n(g)_n}\,z^n \quad (4.7b)$$

$$= B^{-1}(c, g-c)\sum_l\sum_m \frac{(a)_{l+m}(b)_m(d)_l}{(1)_l(1)_m(e)_l(f)_m}\,x^l y^m \times \int_0^1 w^{c-1}(1-w)^{g-c-1}(1-zw)^{-d-l}\,dw \quad (4.7c)$$

$$= B^{-1}(c, g-c)\int_0^1 \sum_l\sum_m \frac{(a)_{l+m}(b)_m(d)_l}{(1)_l(1)_m(e)_l(f)_m}\frac{x}{1-zw}\,y^m \times (w)^{c-1}(1-w)^{g-c-1}(1-zw)^{-d}\,dw \quad (4.7d)$$

$$= B^{-1}(c, g-c)B^{-1}(d, e-d)B^{-1}(b, f-b) \times \int_0^1\int_0^1\int_0^1 u^{d-1}v^{b-1}w^{c-1} \times (1-u)^{e-d-1}(1-v)^{f-b-1}(1-w)^{g-c-1} \times (1-zw)^{-d}\left(1-\frac{xu}{1-zw}-yv\right)^{-a} du\,dv\,dw. \quad (4.7e)$$

It remains to be seen if this integral can be cast into a Radon form.

At this juncture it is appropriate to note that the ${}_2F_1$ function, which appears first in SU_3 at the U_2 *sublevel* as a result of the application of the U_2 operator E_{21}, is a Radon transform over a line segment, the group-theoretic *fundamental region* of U_2. Similarly, in SU_4 we find the F_2 function generated by the lowering operator L_3^1 of the U_3 sublevel, this function again being a Radon transform but now over a triangular plane surface, the *fundamental region* of U_3. These examples are indicative of the connection of such generalized hypergeometric functions to the geometry of U_n. It is our contention that when this connection of the generalized functions to the underlying geometry is clearly established, a true insight shall be gained to the otherwise arbitrary manipulations and generalizations of functions that are of particular importance in physics.

ACKNOWLEDGMENTS

The present paper is a product of discussions with Professor L. C. Biedenharn. I would like to thank him in particular for suggesting a closer look at Eq. (44) of Ref. 7—which lead to the generalization of Young tableaux calculus and the associated combinatorial interpretation—and for indicating the possibility of a connection between these generalized functions and Radon transforms.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Critical-Point Singularities of the Perturbation Series for the Ground State of a Many-Fermion System*

GEORGE A. BAKER, JR., AND JOSEPH KAHANE
Applied Mathematics Department, Brookhaven National Laboratory, Upton, Long Island, New York

(Received 9 August 1968)

We show that the many-fermion ground-state energy with an attractive potential has a critical singularity. This singularity destroys the validity of "low-density" approximations. We also find that the K-matrix formalism is, in principle, not applicable to attractive potentials because of the presence of "Emery singularities." We introduce an R-matrix formalism which is numerically very close to the K matrix and free from manifest "Emery singularities." A model calculation is performed on the lattice gas to try to anticipate what quality of results can be expected from summing an R-matrix expansion with fixed density.

1. INTRODUCTION

In mathematical terms, the problem of the ground-state energy of a many-fermion system, when viewed in the context of perturbation theory, is simply a problem in series summation. All we are in fact given by perturbation theory is a power series in the potential strength. One can break down the contribution to each power in various convenient ways, but it is really only the total contribution to each power which is significant. This series summation problem is complicated by several features. In the first place, the series is very probably divergent and at best asymptotic.[1] In the second place, every term in the series is divergent for infinitely hard-core potentials, which are physically acceptable. So we must resum the series to allow this case to be dealt with. For purely repulsive potentials this resummation has been accomplished in a satisfactory manner by means of the summation of all ladder diagrams. It has been rigorously[2,3] proved that for purely repulsive potentials the ladder energy is free of singularities in the range of strengths $0 < v < \infty$. In the presence of attraction, as we note below, the resummation to treat hard-core potentials is not so simply handled. Finally, the location, or even the existence of singularities, which may occur at various points in the potential strength–density plane, has not received the careful attention it deserves. The location of such singularities is of crucial importance to any program of series summation, as it is well known that the nearest one limits the radius of convergence of a Taylor series. No program which has as its goal the calculation of the ground-state energy of a many-fermion system can hope to be successful until it has taken account of at least the closest such singularities. In particular, it is widely recognized that in many ways nuclear matter, for example, is very much like a liquid drop and that the ground-state energy-vs-density curve should have a flat portion for low density corresponding to a condensed nucleus which does not fill the whole volume. The saturation minima obtained by approximate schemes have been represented as analytic continuations of the high-density portion of the curve. *However, the logical consequences of the liquid aspects of the nature of a many-fermion ground state must be taken into account.* (We do this in Sec. 2.) From the theory of liquids and gases we expect, and indeed find, that there will be a potential strength for which the densities of the liquid and gaseous phases of the many-fermion system, interacting through an attractive potential with a strong repulsive core, will become equal and a phase separation will cease to be. At this point, called the critical point, the theory of liquids and gases (and of cooperative phenomena in general) tells us there is *an analytic singularity*. This situation is in sharp contrast to the situation for a purely repulsive potential, where a low-density expansion[4] proves to be satisfactory because of the absence of a liquid–gas critical-point singularity. The presence of the critical singularity renders inadequate (as in classical statistical mechanics) approximation procedures based on the assumption of low density, since the ground state lies on the liquid side of the coexistence curve. A low-density expansion is blocked off from the liquid side of the coexistence curve by having to pass through the two-phase region, where the curves are flat. On the other hand, if one tries an expansion in terms of the number of interacting particles, which is accurate both for low density and

* Work performed under the auspices of the U.S. Atomic Energy Commission. Preliminary report of part of this work given to the American Physical Society, April 1967. Bull. Am. Phys. Soc. II 12, 594 (1967).

[1] G. A. Baker, Jr., Phys. Rev. 131, 1869 (1963).

[2] G. A. Baker, Jr., J. L. Gammel, and B. J. Hill, Phys. Rev. 132, 1373 (1963); hereinafter called I.

[3] G. A. Baker, Jr., B. J. Hill, and R. J. McKee, Jr., Phys. Rev. A135, 922 (1964); hereinafter called II.

[4] G. A. Baker, Jr., Phys. Rev. 140, B9 (1965); hereinafter called III.

weak interaction, one may again have trouble as the critical-point singularity lies directly between the origin in the density–potential-strength plane and the liquid side of the coexistence curve. We propose a resummed potential-strength expansion at fixed density which will avoid the critical-point singularity. As the necessary calculations on the quantum many-fermion ground-state energy are quite lengthy, we have chosen to illustrate our procedures by some analogous model calculations on the lattice gas. Current theory of critical phenomena indicates that this model has the same type of singularity structure and thus retains the relevant features concerning a critical singularity, two-phase region, and the like. Hence this model should form a proving ground for our proposed method of calculating the many-fermion ground-state energy.

Using available data, we are able to locate the coexistence curve reasonably accurately and to evaluate the free energy (analogous to the ground-state energy) thereon fairly accurately. The outlook is hopeful that sensible results can be obtained with the fewer terms which are likely to be available for the expansion of the energy in the many-fermion problem.

In the third section we investigate other possible singularities. We find that the "Emery singularities,"[5] in principle, fill the k_F-potential-strength plane when there is *any attraction present at all.* We do not believe that these are real singularities in the energy, as ordinary macroscopic-sized systems do not appear to be a close enough approximation to an infinite system to possess them. Rather, they appear to represent an unfortunate choice of a method of summation of a series which is known to be divergent.[1] We introduce an alternate procedure (R matrix) which is numerically very close to the Brueckner[6] K-matrix method, but free from the "Emery singularities."

By analysis of the singularity structure of the R matrix, we predict that ^{3}He does not have a superfluid phase.

2. THE CRITICAL POINT OF A MANY-FERMION SYSTEM

In this section we will be concerned principally with interparticle potentials which have a very strong repulsive core surrounded by a purely attractive potential of finite range and depth. Although we are concerned in this article exclusively with the ground-state energy of a many-fermion system, it is sometimes helpful to understanding to consider a problem in the context of a larger one. This we shall do here by introducing a temperature. The ground state will be recovered in the limit as the temperature goes to zero, with the other relevant variables fixed.

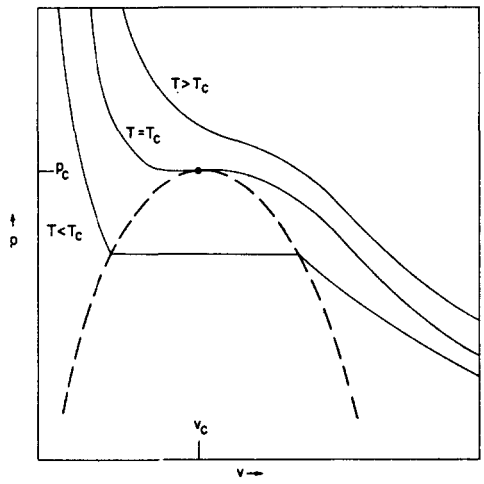


FIG. 1. Sketch of a typical pressure–volume diagram for a liquid–vapor system. The dashed line is the coexistence curve.

Interacting systems with interparticle potentials of the general type we are discussing are quite common in nature and have been much studied. The situation for nuclear matter, the understanding of which is one of the goals of this study, is seemingly unique in that it is a quantal Fermi system whose density is quite low compared to close-packed density. However, we shall argue that these features are merely details and that the reasonable expectation is that nuclear matter will fit into the general picture of cooperative phenomena.

One of the most striking properties exhibited by an extremely wide variety of matter in bulk is that of change of phase—the boiling of water to form steam, for example. This phenomenon occurs at normal atmospheric pressure. As we increase the pressure, the temperature and density of the steam increases; finally, at a *critical point* (p_c, T_c, ρ_c) the density of water and steam become the same, and for higher temperature (or pressure) there is no longer a change of phase.[7]

As one approaches the critical point from (for instance) higher temperature, various manifestations of the impending phase separation appear. A typical p–V diagram is shown in Fig. 1. The dashed line is the coexistence curve. For example, the density fluctuations become very large when a liquid and its vapor are in equilibrium with each other below the critical temperature at the same pressure. (They have different densities. In the absence of gravity one expects to find various droplets of liquid dispersed throughout the volume.) This phenomenon is experimentally

[5] V. J. Emery, Nucl. Phys. **12**, 69 (1959).

[6] See K. A. Brueckner, in *The Many-Body Problem*, C. de Witt, Ed. (John Wiley & Sons, Inc., New York, 1959), pp. 47–154.

[7] For a good recent review of the equilibrium theory of critical phenomena, clearly presented, the reader is referred to M. E. Fisher, Rept. Progr. Phys. **30**, 615 (1967).

manifest as critical opalescence, i.e., the substance becomes cloudy.

Another type of system which displays an exactly analogous behavior is a ferromagnetic crystal near its Curie or critical point where spontaneous magnetization suddenly appears. Here the zero-field magnetic susceptibility becomes infinite at the critical point. One salient feature observed of critical points is that the singular physical behavior is represented by an analytic singularity in thermodynamic properties of these systems. A consequence is that a limit is set on the radius of convergence of ordinary perturbation theory by the existence of such a singularity. Any serious attempt to calculate the properties of many-fermion systems must consider the possibility of such a singularity and take account of it.

The argument that systems such as nuclear matter possess a two-phase region is quite straightforward. We start from the assumption that the many-fermion system is spatially homogeneous and that the energy is an analytic function of the density; then we show that this assumption leads to a contradiction. Consider a potential with a hard core plus an attractive part of strength, $\lambda = 1 - \epsilon$, $\epsilon > 0$, where $\lambda = 1$ is the strength required to produce a two-body bound state of zero energy. We will suppose that the pair-interaction volume is much larger than the hard-core volume. (In the nuclear case the range of interaction is at least $2\frac{1}{2}$ times the hard-core diameter[8] or a ratio of more than 15 in volume.)

We can now imagine a configuration in which there are up to six interacting pairs per particle (face-centered cubic arrangement) without an appreciable increase in the kinetic energy per particle. Consequently, we expect to be able to obtain a negative many-body ground-state energy at a suitable density because of the relative many-body enhancement of potential energy over kinetic energy.[9] (This effect is evident in the nuclear case from an examination of the experimental binding energy per particle among the light elements.[10]) However, it has been shown[4,11] that

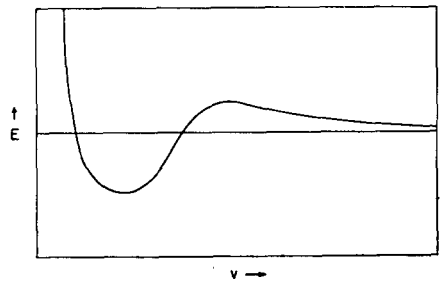


FIG. 2. Sketch of energy vs volume for the ground state of a many-fermion system with attractive forces present.

for very low density

$$\left(\frac{Em}{N\hbar^2}\right) = \tfrac{3}{5}k_F^2 + \frac{1}{3\pi}ak_F^3 + \cdots,$$

where k_F is the Fermi momentum and is proportional to the cube root of the density. Hence the energy is positive at very low density. By choosing $\lambda = 1 - \epsilon$, the scattering length a is finite; although it is infinite for $\lambda = 1$, which would vitiate this argument at that potential, a is finite and analytic for all $0 \leq \lambda < 1$. For high densities the energy per particle becomes indefinitely great as the available amount of attraction per particle is bounded (because of the hard cores and finite range and depth), but the repulsive kinetic energy from restricting the available volume is not. The energy curve for a spatially homogeneous system must look like Fig. 2. We shall assume that the energy curve varies continuously with temperature as T goes to zero for fixed density.[12]

We now use the following rigorous result of statistical mechanics. The Helmholtz free energy (per *particle*) is convex,[13,14]

$$\Psi(T, \tfrac{1}{2}(v_1 + v_2)) \leq \tfrac{1}{2}\Psi(T, v_1) + \tfrac{1}{2}\Psi(T, v_2), \quad (2.1)$$

with continuous derivative for all (nonzero) temperatures. The Helmholtz free energy[15] is defined as

$$\Psi = E - TS, \quad (2.2)$$

where E is the internal energy (per particle), T the absolute temperature, and S the entropy (per particle). Now the entropy per particle[16] diverges to plus infinity like the logarithm of the volume in the limit of large volumes. We may now pick a temperature small enough so that, for all volumes in any given range between a lower limit greater than the jamming volume and less than some finite upper limit, Ψ is

[8] See, for example, J. L. Gammel and R. M. Thaler, Phys. Rev. **107**, 291, 1337 (1957).

[9] A more nearly rigorous proof can be given by dividing space up into equal cubes, each containing, say, 3 or more particles. If we then impose zero boundary conditions along the cube boundaries, we have restricted the class of wavefunctions allowed and hence possibly raised the ground-state energy. If we now drop the attractive intercube interactions and thicken the walls to take account of the intercube repulsive interactions, we reduce our problem to a set of finite problems which give an upper bound to the energy of the complete problem. The application of variational techniques [see, for example, N. Austern and P. Iano, Nucl. Phys. **18**, 672 (1960)] now suffice to establish a negative eigenvalue for some intermediate density.

[10] See, for example, J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1952).

[11] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).

[12] See the proof by J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).

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

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

[15] See, for example, P. S. Epstein, *Textbook of Thermodynamics* (John Wiley & Sons, Inc., New York, 1937).

[16] T. L. Hill, *Statistical Mechanics* (McGraw-Hill Book Co., Inc., New York, 1956).

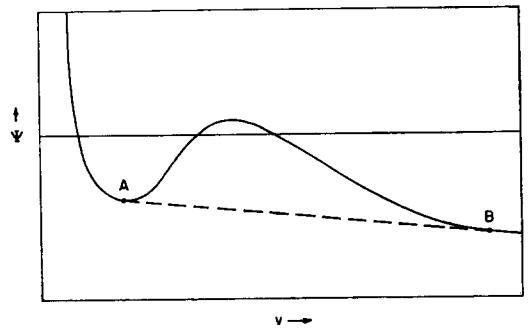


FIG. 3. Free energy vs volume for a low-temperature many-fermion system with attractive forces present. The dashed line is the convex hull or two-phase portion.

within any preassigned distance of E as the entropy is bounded in that range. In the low-density (large-volume) limit for any $T > 0$, however, Ψ tends to $-\infty$ because E is bounded and $S \to +\infty$. This argument establishes a region where Ψ is positive. Therefore, the Helmholtz free energy under these assumptions fails to be convex, which is a contradiction. We conclude that the ground state is not one spatially homogeneous phase. We may, however, construct a convex Ψ by taking the convex hull of the spatially homogeneous Ψ, i.e., by drawing the tangent line across the re-entrant portions, as in Fig. 3. This tangent line is realized by a two-phase system of suitable proportions of spatially homogeneous systems at densities A and B to construct the required intermediate density.

Let us now consider our system at very high temperature. By the correspondence principle,[17] quantum effects become negligible and we may consider classical behavior. The attractive interaction energies, having a finite maximum, become inconsequential compared to the kinetic energies, and hence the possibility of a liquid-vapor-type phase change ceases to exist[18]: if we imagine a liquid droplet formed, the attraction would be too weak to bind a particle having even the average kinetic energy and hence the droplet would immediately evaporate. We concluded, therefore, that, as there is a two-phase region for very low temperature and no two-phase region for very high temperature, there must be a positive least-upper bound to temperatures for which two phases are possible. This temperature we call the critical temperature. Although we recognize that the boundary of the two-phase region could have a flat top (up as in Fig. 1), we will continue to treat the simpler case where the top is a single point, which seems to be the usual circumstance observed in many analogous cases.

Having established the existence of a critical temperature, we may ask how its location varies as a function of the strength of the attractive part of the potential λ. For weaker λ there is less binding energy available and a stronger tendency for droplets to evaporate. Hence the critical temperature decreases as λ decreases. When λ is zero (hard cores only), there is no possibility of a liquid, as a droplet would have no binding energy at all.

This argument implies the convexity of E at $T = 0$ (except for a possible order–disorder transition at higher density). Hence, interpolating between $\lambda = 0$ and Fig. 2, there must be a greatest-lower bound to λ's which have nonconvex E vs v curves under the spatially homogeneous constraint. Consequently, there exists a critical potential $0 < \lambda_c < 1$ for which the critical temperature is exactly zero. There is a corresponding critical density ρ_c (or perhaps a range of densities). The significance of this critical point (λ_c, ρ_c) in the (potential-strength–density) plane for fixed temperature (zero) is, as explained above, the reasonable expectation that it must be an analytic singularity, as is every other known critical point. We defer a discussion of the close similarity of known critical points to Sec. 4.

From the foregoing discussion it is plain that the ground state of such a many-fermion system is a cooperative state which can rightly be considered as a liquid.[19] Approximation procedures based solely on the assumption of a dilute gas-like system are not adequate as the density, rather than being low, is higher than critical density, which is the relevant density for the importance of higher-order cluster interactions.

3. OTHER ANALYTIC SINGULARITIES OF THE GROUND-STATE ENERGY

In a previous paper[4] we argued that the analytic singularity in the energy as a function of potential strength which occurs when two particles are just bound (deutron for the nuclear case) continues to nonzero density and, in fact, forms a monotonically increasing curve in the k_F–λ plane. The analytic structure of the ladder approximation to the energy as a function of potential strength for fixed density was established.[3,4] That such singularities should exist has

[17] E. Wigner, Phys. Rev. **40**, 749 (1932).

[18] There may still be a solid–fluid phase change at high density on account of the hard cores, but we are not presently concerned with this. See D. S. Gaunt and M. E. Fisher, J. Chem. Phys. **43**, 2840 (1965).

[19] For a description of the Bohr liquid drop model of the nucleus, see, for example, R. D. Evans, *The Atomic Nucleus* (McGraw-Hill Book Co., Inc., New York, 1955), Chap. 11, Sec. 3. The successful aspects have long been recognized to be the bulk properties, surface energies, separation energies, etc., which one would expect from either a classical or quantal liquid, which are, of course, just the aspects relevant to the present discussion.

long been recognized.[5,20] The relevant question, in so far as a study of the ground-state energy of a many-fermion system is concerned, is their location (in the k_F–λ plane) relative to the coexistence curve. If none of these singularities lie in the one-phase region, then they are, in principal, no impediment to the calculation of the ground-state energy. If, on the other hand, they intrude into the one-phase region, then they proscribe the calculation of the ground-state energy there. We have argued in the previous section that, for the type of potentials we are considering (see Sec. 2), the many-body effects which enhance the potential relative to the kinetic-energy contributions cause the many-body binding energy per particle to increase when the number of particles in the system does. Consequently, a weaker potential is required to cause a given binding energy per particle for a larger system than for a smaller one. Therefore we expect the two-body bound states which cause singularities in the ladder approximation to occur for stronger potentials than saturation.

We can give significance to the low-density terminology of bound states by a discussion in the presence of a Fermi sea in terms of spatial homogeneity. In the low-density case the normalization of the wavefunction when two particles are close together (in a "bound" state) is proportional to $v^{-\frac{1}{2}}$ (v is volume), instead of $1/v$, as it would be if they were uncorrelated. This region will persist as we increase the density of the surrounding Fermi sea. The effect of the presence of the Fermi sea[21] is to prevent the occurrence of most of the low frequencies in the wavefunction. They[21] say that it "heals" quickly; however, the amplitude of the "healed" (undisturbed frequency) portion of the wavefunction will differ from that of the unperturbed wavefunction when there is a spatially inhomogeneous portion present, as there will be a nonzero fraction of the total normalization in the correlated portion. As the density of the Fermi sea is increased, finally one must use such high frequencies (high kinetic energies) to construct the wavefunction that it becomes energetically unfavorable as compared to the spatially homogeneous state. (See Fig. 4 for the path followed in this argument in the λ–k_F plane.) Since the 3-, 4-, etc., body scattering matrices appear[22] as part of the energy expansion, one finds the same phenomena there as in the two-body case. An analytic singularity will occur in the n-body scattering matrix, where the spatially inhomogeneous case (normalization of the wavefunction when all particles are remote from each other decreases) becomes more favorable than the spatially homogeneous case. If we consider the limit as n becomes infinite for the n-body scattering matrix in a sea of fixed density, the location of the singularity will be the coexistence curve—as the breakdown of spatial homogeneity (one phase) is the *definition* of a liquid–vapor coexistence curve. Consequently, we conclude that the coexistence curve is a limit point of singularities of subsequences which occur in the complete energy. Fortunately, as we have discussed above, the limit, for potentials of the sort we are treating, is approached from the more strongly attractive side, and we are not barred, in principle, from computing the energy on the coexistence curve from the less strongly attractive side.

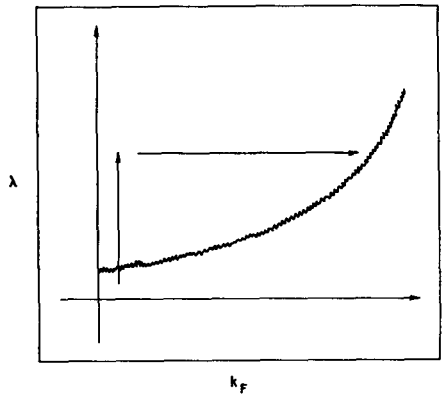


FIG. 4. Path in the $\lambda - k_F$ plane which leads to the occurrence of a spatially inhomogeneous (two-body) portion of the many-body wavefunction. The jagged line is a line of singularities (fixed l).

Whether or not the coexistence curve is a line of singularities of the analytic function

$$\hat{E}(k_F, \lambda) = \sum_{n=0}^{\infty} \lim_{N\to\infty} {}_N e_n \lambda^n, \tag{3.1}$$

as well as

$$E_\infty(k_F, \lambda) = \lim_{N\to\infty} \sum_{n=0}^{\infty} {}_N e_n \lambda^n, \tag{3.2}$$

is clearly of crucial importance to any attempt to compute the energy on the coexistence curve. Katsura[23] has examined a classical model and shown that, in spite of Yang and Lee's[24] results on (3.2), it is doubtful whether the singularity of (3.1) coincides with the irregular point of (3.2). One of us[25] has given numerical evidence to indicate that, except at the critical point itself, the coexistence curve does not contain singularities of (3.1) at least for the nearest-neighbor, Ising-model lattice gas. Katsura[26] has gone

[20] R. Balian, *The Many-Body Problem*, C. Fronsdal, Ed. (W. A. Benjamin, Inc., New York, 1962), p. 286.
[21] L. C. Gomez, J. D. Walecka, and V. F. Weisskopf, Ann. Phys. (N.Y.) **3**, 241 (1958).
[22] H. A. Bethe, Phys. Rev. **138**, B804 (1965).
[23] S. Katsura, Progr. Theoret. Phys. (Kyoto) **11**, 476 (1954); **23**, 390 (1960), and references therein.
[24] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404, 410 (1952).
[25] G. A. Baker, Jr., Phys. Rev. **161**, 434 (1967).
[26] S. Katsura, Progr. Theoret. Phys. (Kyoto) **13**, 571 (1955); also see his review article Advan. Phys. **12**, 391 (1963).

even further for the long-range, Huisimi–Temperley model and proved that the coexistence curve is not a line of singularities. Saito[27] shows that the singularities of (3.1) very likely correspond to the end of supersaturation. By a method of an electrostatic analog with the use of image charges, he demonstrates for the Huisimi–Temperley model that the critical point is the only singularity on the coexistence curve. This result is in accord with our numerical results mentioned above for a different model.

To illustrate these results we have calculated the ladder approximation to the energy by the usual methods.[2] The location of the singularities are determined as the nearest zero of the determinant of the matrix approximation to the integral equation [Eq. (5.9) of I] for the wavefunction. This zero will be an approximation of the edge of the cut derived previously [Eq. (4.18) of III].

In order to locate which values of the parameters correspond to the singularity, we start with a differential form of the K-matrix equation [(3.8) subject to (3.3) of II]:

$$[H_r + \lambda V]\omega = \mathbf{k}^2\omega \tag{3.3}$$

with H_r the relative coordinate kinetic energy and V the potential energy when the wavefunction ω must be expanded in terms of

$$\exp[i\mathbf{k}\cdot\mathbf{r}],$$
$$|\tfrac{1}{2}\mathbf{p} + \mathbf{k}| > k_F, \quad |\tfrac{1}{2}\mathbf{p} - \mathbf{k}| > k_F. \tag{3.4}$$

The $\mathbf{p}$ and $\mathbf{k}$ are given in terms of the two-hole momenta $\mathbf{m}$ and $\mathbf{n}$ as

$$\mathbf{k} = \tfrac{1}{2}(\mathbf{m} - \mathbf{n}), \quad \mathbf{p} = \mathbf{m} + \mathbf{n}. \tag{3.5}$$

Inspection of (3.3)–(3.5) reveals that the smallest energy gap between the right-hand side of (3.3) and the smallest $|\mathbf{k}|$ allowed by (3.4) to be closed by the attractive part of the potential to form a "bound" state occurs when

$$|\mathbf{m}| = |\mathbf{n}| = k_F. \tag{3.6}$$

Hence the usual K-matrix equation (in terms of a coordinate-space wavefunction) becomes[2]

$$u_{kl}(r) = j_l(kr) - \frac{2}{\pi}\int_0^\infty G_{kl}(r, r')V(r')u_{kl}(r')(r')^2\,dr', \tag{3.7}$$

where, for condition (3.6),

$$G_{kl}(r, r') = \int_k^{k_F+(k_F^2-k^2)^{\frac{1}{2}}} \frac{k''\,dk''}{2(k_F^2 - k^2)^{\frac{1}{2}}} j_l(k''r)j_l(k''r') + \int_{k_F+(k_F^2-k^2)^{\frac{1}{2}}}^\infty \frac{k''^2\,dk''}{k''^2 - k^2} j_l(k''r)j_l(k''r'). \tag{3.8}$$

[27] N. Saito, J. Chem. Phys. **35**, 232 (1961).

The limit as $k \to k_F$ requires special attention. In fact, we will find it necessary to reorganize the summation of the energy series on this account. In addition to the clustering-type singularities previously mentioned, there also occur "Emery singularities." Emery has shown[5,28] that a singularity occurs when

$$\langle k_F|\, v\,|\psi\rangle = 0, \tag{3.9}$$

where ψ is the solution of an integral equation with $G_{kl}(r, r')$ replaced by [Eq. (42) of Ref. 5]

$$\mathbf{F} = \mathbf{G} + \frac{\langle k_F|\, v\mathbf{G}v\,|k_F\rangle}{|\langle k_F|\, v\,|k_F\rangle|^2}|k_F\rangle\langle k_F| - \frac{\mathbf{G}v\,|k_F\rangle\langle k_F|}{\langle k_F|\, v\,|k_F\rangle} - \frac{|k_F\rangle\langle k_F|\, v\mathbf{G}}{\langle k_F|\, v\,|k_F\rangle},$$
$$|\psi\rangle = |k_F\rangle - \mathbf{F}v\,|\psi\rangle, \tag{3.10}$$

where

$$\langle r|\,\mathbf{G}\,|r'\rangle = \frac{2}{\pi}\int_{k_F}^\infty dk\,\frac{k^2 j_l(kr)j_l(kr') - k_F^2 j_l(k_F r)j_l(k_F r')}{k^2 - k_F^2} \tag{3.11}$$

and $|k_F\rangle = j_l(k_F r)$. These singularities of the ladder series, in general (for the type of potential we are considering), occur for weaker potentials than do the clustering type ($k = 0$). In the low-density limit, (3.9) corresponds to[28]

$$\tan\delta_l(k_F) = 0, \tag{3.12}$$

where δ_l is the phase shift of the corresponding Schrödinger equation. If we use a potential

$$\begin{aligned} v &= +\infty, \quad r < c, \\ &= -W, \quad c < r < d, \\ &= 0, \quad d < r, \end{aligned} \tag{3.13}$$

then it is easy to compute asymptotically for l large that

$$\tan\delta_l(k) \propto -\frac{d^2Wm}{(2l+3)\hbar^2} + \left(\frac{c}{d}\right)^{2l+1}\left[2l + 1 + \frac{1}{2}\frac{d^2Wm}{\hbar^2}\right]. \tag{3.14}$$

For large l the first term dominates as $c < d$, forcing $\tan\delta_l(k)$ negative *no matter how weak W may be.* Thus, at low density the ladder series has an "Emery singularity" for l large enough with any attractive force at all. We have followed these singularities numerically to higher density, and while they move to stronger potentials with increasing density, as we expect, there is always another for high enough l so

[28] V. J. Emery, Nucl. Phys. **19**, 154 (1960).

that the entire attractive potential region of the (k_F, λ) plane is filled with "Emery singularities" of the ladder series.

However, these results do not tell the whole story. If we examine the rate of approach of the potential $V_s(k)$ for which we have a singularity to $V_s(k_F)$, we find that

$$V_s(k) \sim V_s(k_F) - \omega/[\log(1 - k/k_F)]. \quad (3.15)$$

As l increases, so does ω. The region in which $V_s(k)$ is lower than $V_s(0)$ is very tiny.

For example, from the relation between k_F and the volume per particle we can compute that the average level spacing is

$$dN/dk_F = 3N/k_F,$$

and hence we expect, for a macroscopic sample, that the smallest that the argument of the log in (3.15) can be is about 10^{-24}. We have computed the singularity curve of the K matrix for a potential with a hard core and attractive square well [see Eq. (3.43) below] for $b = 4a$. In that case for $l = 0$, $k_F = 1.0$, $V_s(0) \sim 4.3$, there is a maximum near $k/k_F = 0.7$ of $V_s(0.7) \sim 10.2$ and $V_s(1) = 3.2$. However, for a macroscopic-sized system $V_s(1 - 10^{-24}) \sim 4.0$, *a long way* from the limit as $k \to k_F$! As l increases, the strength of potential needed to cause a singularity is generally more attractive, except for $k = k_F$, where, as we saw, it is less so. The region around $k = k_F$, where $V_s(k)$ is less than $V_s(0)$, decreases in size very rapidly. It is hard to ascribe much relevance in the physical world to a phenomenon which seems to require a much vaster than normal macroscopic-sized system for its existence.

Brueckner and Gammel[29] made the simple approximation of adding a small excitation energy to the denominator of the Green's function [our Eq. (3.8), for example] as a numerical expedient to prevent an infinity in their numerical work. We have checked that this procedure has the effect of moving $V_s(k_F)$ well above (in most of the type of cases we are considering) $V_s(0)$.

We know very well that for certain potential shapes (potential of one sign) the energy is indeed singular in the presence of any attraction at all—the well-known nuclear collapse problem. This consideration suggests to us that the ladder series may be giving a "shape-independent" approximate description of the nuclear collapse phenomenon. For the potentials we are considering, we know that it is the "excluded-volume" effect of the hard cores in the many-body problem which prevents this collapse. (In any event, it does not seem relevant to the size of systems we are attempting to treat.) We therefore conclude that a different summation procedure than those based on the K matrix is required to make a valid singularity-free calculation of the many-body energy.

We propose to rearrange the energy series in powers—not of Brueckner's K matrix as has been done, but in powers of a closely related matrix which we will call R. The reason that the ordinary potential-strength expansion was rearranged into powers of K was to enable one to treat potentials with an infinite repulsive core. This feature must clearly be retained. The usual K matrix (in ladder approximation) is given by (5.7), (5.9), and (5.10) of I. They are

$$K_l(k) = \frac{2}{\pi}\int_0^\infty j_l(kr)V(r)u_{kl}(r)r^2\,dr, \quad (3.16)$$

where

$$u_{kl}(r) = j_l(kr) - \frac{2}{\pi}\int_0^\infty G_{kl}(r, r')V(r')u_{kl}(r')r'^2\,dr' \quad (3.17)$$

and

$$G_{kl}(r, r') = \int_0^\infty k''^2\,dk''\frac{j_l(k''r)j_l(k''r')}{k''^2 - k^2}F(p, k'') \quad (3.18)$$

with p the center-of-mass momentum, k the relative momentum, $j_l(x)$ the usual spherical Bessel functions, and $F(p, k'')$ a function which represents the effect of the Pauli exclusion principle. The low-density limit of the many-body energy

$$\Delta E = \frac{3}{(2\pi k_F)^3}\iint_{\substack{|\frac{1}{2}\mathbf{p}+\mathbf{k}|\le k_F \\ |\frac{1}{2}\mathbf{p}-\mathbf{k}|\le k_F}} dk\,dp \times \sum_l (2l+1)\begin{pmatrix}1 & l & \text{even}\\ 3 & l & \text{odd}\end{pmatrix}K_l(k) \quad (3.19)$$

has been shown[4,11] to be proportional to the scattering length

$$a = \tan\delta_0(0) = \int_0^\infty V(r)u_{00}(r)r^2\,dr. \quad (3.20)$$

This result corresponds to the standing-wave normalization for the wavefunction.[6,30]

If we introduce the Green's function

$$\mathcal{G}_{kl}(r, r') = \int_0^\infty dk''\frac{[k''^2 j_l(k''r)j_l(k''r') - k^2 j_l(kr)j_l(kr')]}{k''^2 - k^2}, \quad (3.21)$$

then there is no singularity in the integrand at $k'' = k$. We may, following usual procedures,[30] evaluate (3.21). It is

$$\mathcal{G}_{kl}(r, r') = -kj_l(kr_<)n_l(kr_>), \quad (3.22)$$

[29] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958).

[30] T. Y. Wu and T. Ohmura, *Quantum Theory of Scattering* (Prentice-Hall, Inc., Englewood Cliffs, N.J., 1962).

where $r_<$ and $r_>$ are the lesser and greater of r and r', respectively. This is exactly the standing-wave[30] Green's function. The form (3.21) is well defined for all k's and is also suitable for the inclusion of the Pauli exclusion principle. We therefore introduce

$$\tilde{G}_{kl}(r, r') = \int_0^\infty dk'' \frac{[k''^2 j_l(k''r) j_l(k''r') - k^2 j_l(kr) j_l(kr')]}{k''^2 - k^2} F(p, k'') + \tilde{a}(p, k) j_l(kr) j_l(kr'). \quad (3.23)$$

Form (3.23) of $\tilde{G}$ can now be well defined for all k and p, not just those in the Fermi sea as was the case for (3.18), by extending the definition of $F(p, k'')$ to be

$$\begin{aligned} F(p, k'') &= 1, \quad \tfrac{1}{2}p - k_F > k'', \\ &= 0, \quad (k''^2 + \tfrac{1}{4}p^2)^{\frac{1}{2}} < k_F, \\ &= 1, \quad k'' - \tfrac{1}{2}p \geq k_F, \\ &= \frac{k''^2 + \frac{1}{4}p^2 - k_F^2}{k''p}, \quad \text{otherwise.} \end{aligned} \quad (3.24)$$

The second term $\tilde{a}(p, k)$ is arbitrary provided it vanishes when k_F does. We choose $\tilde{a} = k^2/k_F$ ($k < k_F$) as a simple function which minimizes the difference between $\tilde{G}$ and G.

We wish to expand the solution of (3.17) in terms of the solution of

$$\tilde{u}_{kl}(r) = j_l(kr) - \frac{2}{\pi}\int_0^\infty \tilde{G}_{kl}(r, r') V(r') \tilde{u}_{kl}(r') r'^2 \, dr'. \quad (3.25)$$

To do this, we observe that (3.17) can be rewritten as

$$u_{kl}(r) = A j_l(kr) - \frac{2}{\pi}\int_0^\infty \tilde{G}_{kl}(r, r') V(r') u_{kl}(r') r'^2 \, dr', \quad (3.26)$$

where

$$A = 1 + \frac{2}{\pi}\left[\int_0^\infty \frac{k^2 \, dk''}{k''^2 - k^2} F(p, k'') - \tilde{a}(p, k)\right] \times \left[\int_0^\infty j_l(kr') V(r') u_{kl}(r') r'^2 \, dr'\right]. \quad (3.27)$$

Thus, solving for A, we get

$$A = \left[1 + \frac{1}{\pi}(\tau_1 - 2\tilde{a})\int_0^\infty j_l(kr') V(r') \tilde{u}_{kl}(r') r'^2 \, dr'\right]^{-1} \quad (3.28)$$

where we use the notation of III:

$$\tau_1 = 2\int_0^\infty \frac{k^2 \, dk''}{k''^2 - k^2} F(p, k''). \quad (3.29)$$

Hence,

$$u_{kl}(r) = A \tilde{u}_{kl}(r) \quad (3.30)$$

and

$$K_l(k) = \frac{R_l(k)}{1 + (\frac{1}{2}\tau_1 - \tilde{a}) R_l(k)}, \quad (3.31)$$

where we define the diagonal elements of the R matrix as

$$R_l(k) = \frac{2}{\pi}\int_0^\infty j_l(kr) V(r) \tilde{u}_{kl}(r) r^2 \, dr. \quad (3.32)$$

The Emery singularity arises in (3.31) if $R_l < 0$, as τ_1 can be arbitrarily large. From (3.31) the expansion of $K_l(k)$ in powers of the R matrix is quite straightforward:

$$K_l(k) = R_l(k) - (\tfrac{1}{2}\tau_1 - \tilde{a}) R_l^2(k) + (\tfrac{1}{2}\tau_1 - \tilde{a})^2 R_l^3(k) + \cdots. \quad (3.33)$$

If we substitute (3.33) into (3.19), then, as τ_1 diverges only logarithmically, the integral of every power is convergent; hence the expansion of ΔE (ladder) is well defined in powers of the R matrix, provided R itself is defined. The coefficients of the expansion, of course, are divergent like $(n!)$. This divergence is the same as that for K in powers of V[1]. This similarity in divergence rates follows from the fact that, as $\tilde{G}(r, r')V(r')$ is bounded for $V(r)$ bounded and of finite mass, R must have a finite radius of convergence when expanded in powers of the potential strength. In the low-density limit we see that R has the standing-wave singularity of $\tan \delta_l(k)$. These are well known to correspond to the occurrence of a two-body bound state.

To inquire whether the complete energy series can be resummed by this procedure, we have examined the K-matrices which result from the ladder-type insertions to convert all possible types of V vertices (see Fig. 2 of Ref. 1) into K vertices. They can be divided into two relevant categories. The first category comprises those in which the higher-order ladder insertions either begin or end with an E or F vertex (number of excited states changes by ± 2). In this situation Hugenholtz[31] has shown that the sum over all "time orders" gives an effective denominator which has no contribution from the excitation of the Fermi sea. Here we require only nondiagonal K matrices, which can be obtained as

$$\langle k' | K_l | k \rangle = \frac{\langle k' | R_l | k \rangle}{1 + (\frac{1}{2}\tau_1 - \tilde{a}) R_l(k)}, \quad (3.34)$$

where we define

$$\langle k' | R_l | k \rangle = \frac{2}{\pi}\int_0^\infty j_l(k'r) V(r) \tilde{u}_{kl}(r) r^2 \, dr \quad (3.35)$$

[31] N. M. Hugenholtz, in *The Many-Body Problem*, C. de Witt, Ed. (John Wiley & Sons, Inc., New York, 1959), pp. 1–46.

and the expansion of (3.34) is analogous to that of (3.33). The other category comprises all the others. For these the denominators include an excitation of the Fermi sea. The integral equation for the K-matrix wavefunction is now (3.17), but with

$$G_{kql}(r, r') = \int_0^\infty k''^2\, dk'' \frac{j_l(k''r) j_l(k''r')}{k''^2 - k^2 + q^2} F(p, k'', k, q) \tag{3.36}$$

instead of (3.18). The Pauli-principle function is such that the denominator is nonnegative definite where $F \neq 0$; however, $k^2 - q^2$ may be positive or negative. To handle these cases we introduce

$$\begin{aligned}\tilde{G}_{kql}(r, r') &= \int_0^\infty dk'' \frac{k''^2 j_l(k''r) j_l(k''r')}{k''^2 - k^2 + q^2} F(p, k'', k, q) \quad \text{if} \quad q^2 \geq k^2, \\ &= \int_0^\infty dk'' \frac{\{k''^2 j_l(k''r) j_l(k''r') - (k^2 - q^2) j_l[(k^2 - q^2)^{\frac{1}{2}} r] j_l[(k^2 - q^2)^{\frac{1}{2}} r']\}}{k''^2 - k^2 + q^2} F(p, k'', k, q) \\ &\quad + \tilde{a}(p, k, q) j_l[(k^2 - q^2)^{\frac{1}{2}} r] j_l[(k^2 - q^2)^{\frac{1}{2}} r'] \quad \text{if} \quad k^2 > q^2. \end{aligned} \tag{3.37}$$

Then, if we define

$$\begin{aligned}\langle k' | R_1 | k \rangle &= \int_0^\infty j_l(k'r) V(r) \xi_{k,q,l}(r) r^2\, dr, \\ \langle k' | R_2 | (k^2 - q^2)^{\frac{1}{2}} \rangle &= \int_0^\infty j_l(k'r) V(r) \eta_{k,q,l}(r) r^2\, dr, \end{aligned} \tag{3.38}$$

where

$$\begin{aligned}\xi_{kql}(r) &= j_l(kr) - \int_0^\infty \tilde{G}_{kql}(r, r') V(r') \xi_{kql}(r') r'^2\, dr', \\ \eta_{kql}(r) &= i_l[(k^2 - q^2)^{\frac{1}{2}} r] \\ &\quad - \int_0^\infty \tilde{G}_{kql}(r, r') V(r') \eta_{kql}(r') r'^2\, dr', \end{aligned} \tag{3.39}$$

for the wavefunction corresponding to (3.36) we can write

$$\begin{aligned} u_{kql}(r) &= \xi_{kql}(r) \\ &\quad - \frac{\eta_{kql}(r) \langle (k^2 - q^2)^{\frac{1}{2}} | R_1 | k \rangle L(p, k, q)}{1 + L(p, k, q) \langle (k^2 - q^2)^{\frac{1}{2}} | R_2 | (k^2 - q^2)^{\frac{1}{2}} \rangle}, \end{aligned} \tag{3.40}$$

where

$$\begin{aligned} L(p, k, q) &= \int_0^\infty \frac{(k^2 - q^2)}{k''^2 - k^2 + q^2} F(p, k'', k, q)\, dk'' - \tilde{a}, \quad k^2 > q^2, \\ &= 0, \quad k^2 \leq q^2. \end{aligned} \tag{3.41}$$

Hence

$$\begin{aligned} &\langle k' | K_q | k \rangle \\ &= \langle k' | R_1 | k \rangle \\ &\quad - \frac{\langle k' | R_2 | (k^2 - q^2)^{\frac{1}{2}} \rangle \langle (k^2 - q^2)^{\frac{1}{2}} | R_1 | k \rangle L(p, k, q)}{1 + L(p, k, q) \langle (k^2 - q^2)^{\frac{1}{2}} | R_2 | (k^2 - q^2)^{\frac{1}{2}} \rangle}, \end{aligned} \tag{3.42}$$

which leads directly to an expansion of K_q in powers of R_2. The Emery singularities are here seen to be associated with $\langle (k^2 - q^2)^{\frac{1}{2}} | R_2 | (k^2 - q^2)^{\frac{1}{2}} \rangle = 0$, which are analogous to those for an unexcited Fermi sea.

We now turn to an investigation of the singularity structure of the R matrix. We have computed the smallest positive zeros in λ of the determinant of (3.25) for the potential

$$\begin{aligned} V(r) &= 10^5, && 0 \leq r < a, \\ &= \tfrac{1}{2}(V(a^+) + V(a^-)), && r = a, \\ &= -\pi^2 a^2/(2(b - a))^2, && a < r \leq b, \end{aligned} \tag{3.43}$$

where we have used $b = 4a$ and $b = 2a$. The results are presented in Figs. 5–8. The reader will note in Figs. 5, 6, and 7 the location of singularity in the R matrix. We have argued that this singularity should, in an n-particle cluster in the limit as n becomes

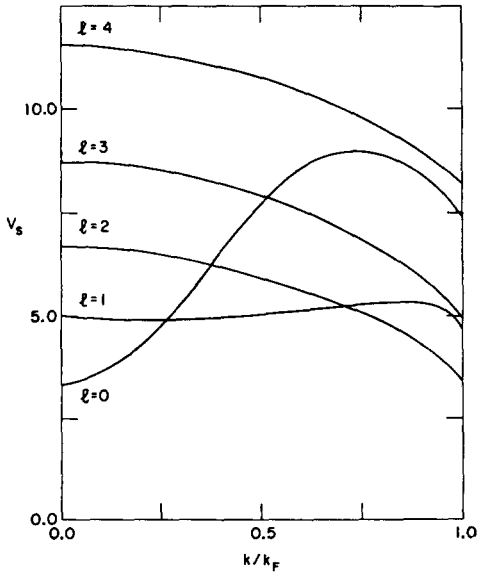


FIG. 5. The potential strength V_s corresponding to the closest singularity of R plotted as a function of k/k_F for $k_F = 0.75$ for the potential (3.43) with $b = 4a$. The curves are for different values of the angular momentum l.

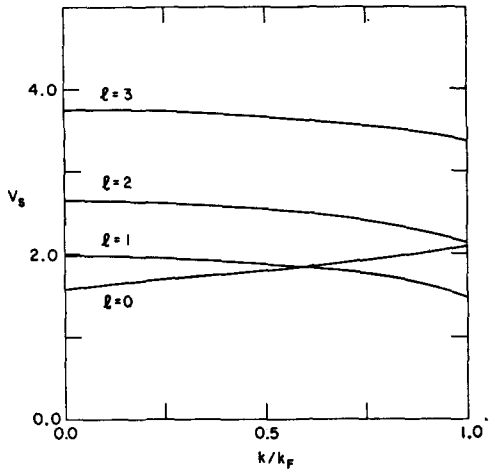


FIG. 6. The potential strength V_s corresponding to the closest singularity of R plotted as a function of k/k_F for $k_F = 0.75$ for the potential (3.43) with $b = 2a$. The curves are for different values of the angular momentum l.

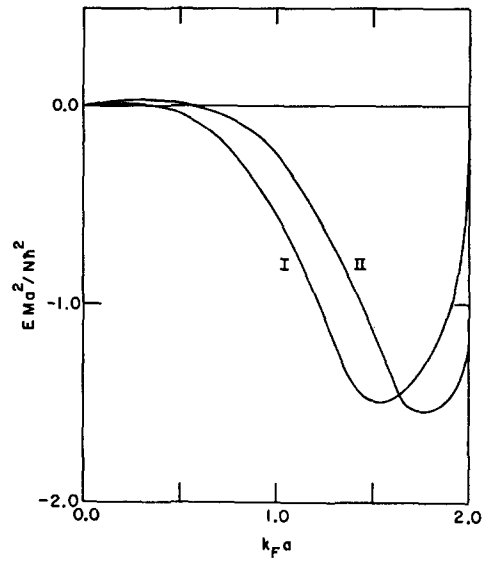


FIG. 8. The energy as a function of k_F in R-matrix approximation. Curve I is potential (3.43) with $b = 4a$ and $\lambda = 1$; curve II is potential (3.43) with $b = 2a$ and $\lambda = 1$.

infinite, approach the saturation minimum. We interpret this discrepancy as an indication that interacting pairs are still a far from adequate description of the infinite case. We have, as a check on the reasoning after (3.5), also, of course, computed throughout the interior of the Fermi sea by the usual procedures[2] as applied, however, to (3.25). All the mesh spacing is the same as in I, except we have used an r mesh of $0.05b$ for a total of 20 points.

Clearly, potentials of the form we have been discussing are not the only interesting possible forms. If we place an electron in a polarizable lattice, the positively charged lattice distorts to surround the electron with positive charges. Beyond this is left a band of surplus negative charges.[32] If a second electron is introduced, it will experience at close distances repulsion, followed by attraction, followed again by repulsion. These considerations lead us to also consider potentials of the form

$$\begin{aligned} Ma^2V(r)/\hbar^2 &= 10^5, && 0 \le r < a, \\ &= -2.7697663 + \tfrac{1}{2}10^5, && r = a, \\ &= -5.5395326, && a < r < 2a, \\ &= -1.3848832, && r = 2a, \\ &= 2.7697663, && 2a < r \le 4a, \end{aligned} \tag{3.44}$$

which just has a bound state of energy zero.

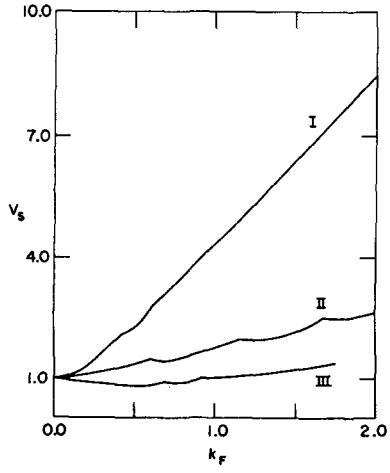


FIG. 7. The potential strength corresponding to the closest singularity of R plotted as a function of k_F. Curve I is potential (3.43) with $b = 4a$; curve II is potential (3.43) with $b = 2a$; curve III is potential (3.44).

We show in Figs. 7 and 9 the location of the singularities and the R-matrix approximation to the energy. [We remark that the K-matrix energy very likely exists for this type of potential, as can be seen from calculations analogous to (3.14).] There is no sign of many-body saturation. The physical reason is simply that two-body pairs are easier to form than many-body clusters because in the many-body clusters the long-range repulsion raises the energy too much. Consequently, the two-body scattering-matrix singularity lies *above* that of the "normal" ground state and prevents its calculation by perturbation theory. It is just this sort of inversion of the singularities of $E(\lambda, k_F)$ which allows a differently organized ground state from the "normal" one and permits the existence of superconductivity and superfluidity. In terms of this type of understanding (i.e., in terms of the coordinate-space potential) and as the He–He interaction[33] can be satisfactorily fitted without a longer-range repulsion (nor has anyone, to our knowledge, suggested that it should have a longer-range repulsion)

[32] J. Friedel, Advan. Phys. 3, 446 (1954).
[33] S. Y. Larsen, Phys. Rev. 130, 1426 (1963).

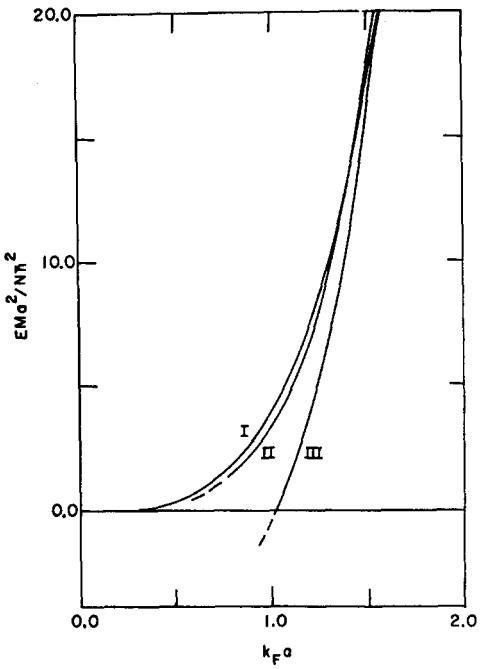


FIG. 9. The energy as a function of k_F in R-matrix approximation. Curve I is for $V = 0.75$ and starts at $k_F = 0$; curve II is for $V = 0.85$. There is a small positive portion $0 \leq k_F a \leq 0.25+$, and then it starts again for $k_F a < 0.75$. The missing portion results from the dip in Fig. 7. Curve III starts at $k_F a < 1.25$. The other values are excluded by the singularities shown in Fig. 7.

we predict that ^{3}He *does not* have a superfluid phase, contrary to the suggestions of some.[34–36] We note that, in fact, Pitaevskii[34] only argues that the exciton–exciton interaction is attractive for large momenta and distances. However, since the system is quantal and not classical, this result is only necessary and not sufficient for the formation of Cooper pairs (leaving other considerations aside). Brueckner *et al.*[35] explicitly assume (with Bardeen, Cooper, and Schrieffer[37]) that the effective interaction potential is a very narrow function in momentum space. This behavior corresponds to an oscillating potential in coordinate space. As we have explained above, this approximation is not too unreasonable for an electron in a polarizable lattice, but the physically essential feature is lacking in the He–He interaction. The calculation of Emery and Sessler[36] cannot be relied on, because they have not produced a solution to the minimization of the free energy for their model Hamiltonians. They have not, as they say, used their Eq. (10) to calculate a consistent form of the effective energy spectrum. If this procedure is used, rather than an experimental value deduced from the physical system as a whole, then the nature of their fundamental equation (14) appears to change rather dramatically.

We remark that there may well be other singularities implicit in the energy series, since the subsequences we have considered do not by any means exhaust all the terms of that series. It is even possible (though we do not think so because of the physical interpretation) that the singularities corresponding to two-, three-, $\cdots$, body binding which we have found are canceled by other terms in the series—although as $\tilde{a}$ is arbitrary, we may not have accurately located them.

4. MODEL THEORIES

In view of our arguments in a previous section (that the ground state of a many-Fermion system interacting through a potential with a repulsive core and short-range attraction must be viewed as a cooperative liquid–vapor system possessing a critical point) and in view of recent results[38] on scaling laws (arguing the detailed universal behavior of properly reduced critical phenomena going in scope and detail beyond the familiar law of corresponding states[15]), it seems natural to turn our attention to more mathematically tractable model theories in order to assess the practicality of various procedures for the calculation of many-Fermion ground-state saturation properties. The results of scaling laws also receive wide experimental[38–40] confirmation and, while they lack some details,[1] yet they clearly give an excellent first approximation. The classical methods of studying liquid-vapor systems have recently been surveyed by Levesque[41]—in particular, the integral-equation approach. He finds, among other things, that in the region of the liquid coexistence curve (just the region we are interested in) none of the equations proposed so far is satisfactory. The procedures which have been successful so far have been Monte Carlo ones.

The computation of the internal energy by various integral equation methods is reasonably accurate, but the computation of the pressure (and hence the location of the coexistence curve) is very poor.

The most straightforward approach to the many-body problem is that of Brueckner.[6] He shows that the expansion in the interaction potential may be re-expressed in terms of an expansion in powers of K, the two-body scattering matrix. The advantage is that

[34] L. P. Pitaevskii, Zh. Eksp. Teor. Fiz. **37**, 1794 (1959) [Sov. Phys.—JETP **10**, 1267 (1960)].
[35] K. A. Brueckner, T. Soda, P. W. Anderson, and P. Morel, Phys. Rev. **118**, 1442 (1960).
[36] V. J. Emery and A. M. Sessler, Phys. Rev. **119**, 43 (1960).
[37] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[38] For a review see L. P. Kadanoff *et al.*, Rev. Mod. Phys. **39**, 395 (1967).
[39] M. S. Green, M. Vicentini-Missoni, and J. M. H. L. Sengers, Phys. Rev. Letters **18**, 1113 (1967).
[40] P. Heller, Rept. Progr. Phys. **30**, 731 (1967).
[41] D. Levesque, Physica **32**, 1985 (1966).

hard-core potentials leave K finite and, hence, not *a priori* intractable in perturbation theory. (We have seen previously[3] that it is likely that an analytic singularity exists in an expansion in terms of λK at $\lambda = 1$, the hard-core point, but it may not necessarily prevent calculation.) We do not consider Brueckner's[6] further resummation of "self-energy" terms for reasons brought out before.[2] [The treatment of the "off-energy shell" propagation is such that the opposite sign is obtained for the correction to the fourth-order (the first order in which this approximation appears) ladder diagram for low density. This error severely affects the numerical content of the Brueckner theory.] The idea has gained currency that the K-matrix expansion is a low-density one[4,42–46]; however, as we have seen above, the existence of the two-phase region in the $(\lambda$–$k_F)$ plane means that an approach based on a low-density basis alone could not be expected to be valid. This situation is in marked contrast to the case of purely repulsive forces, where it has been found[4] to be a good one.

In our opinion a more fruitful viewpoint is the analog between the K expansion (modified by us as the R expansion) and the classical Mayer f expansion articulated by Bloch,[47] who has also extended the work to nonzero temperature. We define

$$f(r) = e^{-\beta V(r)} - 1, \tag{4.1}$$

where $V(r)$ is the classical interaction energy and $\beta = 1/kT$. The configurational part of the partition function is

$$\begin{aligned} e^{-\beta \Sigma V(r_{ij})} &= \prod \{1 + \lambda f(r_{ij})\} \\ &= 1 + \lambda \sum f(r_{ij}) + \lambda^2 \sum ff + \cdots \end{aligned} \tag{4.2}$$

for $\lambda = 1$; hence, all the various thermodynamic properties can also be so expanded. We have defined (analogous to Brueckner's[6] K) the R matrix as

$$R = V - V\tilde{G}R, \tag{4.3}$$

where V is the two-body interaction matrix and $\tilde{G}$ the Green's function with the Pauli-principle effects of the Fermi sea included. Some of the points of analogy between f and R expansions are: Both are selective resummations of the expansion in terms of the interaction potential; both treat the case of infinite repulsive potentials without the introduction of explicit infinities; both give the low-density limit from the first term of the expansion; both *can* (though they are not always used in this way) start from the noninteracting state of a given (nonzero) density as the basis of the perturbation expansion. The expansions differ in the details of the system studied (classical at finite temperature as a function of λ/kT vs quantum at zero temperature as a function of $\lambda Mc^2/\hbar^2$), but, as we pointed out above, there is great similarity in the critical behavior of a wide range of systems. It can be argued also that the zero-point energy of a Fermi system acts much as a temperature. We, of course, recognize that model calculations are useful only in so far as they extract the salient features; we have not demonstrated that this is so, but rather present it as a classical context in which to view the many-fermion problem with attractive potentials.

We choose as our model the lattice gas introduced by Yang and Lee.[24] This model, briefly, is for the configurational part of the partition function. The gas atoms are constrained to sit on the sites of a space lattice, no more than one per site. The adjoining atoms can have an attractive interaction energy. The series we mentioned above and related ones have been much studied.[48,49]

The most extensive data available are those of Rushbrooke and Scoins[50] for open lattices for the Ising model. They define two quantities

$$\ln \Lambda = \rho\left(1 - \sum_{k\geq 1} \frac{k}{k+1}\beta_k \rho^k\right), \tag{4.4}$$

$$\ln \alpha = \ln \rho - z \ln \eta - \sum \beta_k \rho^k, \tag{4.5}$$

where z is the lattice coordination number, ρ the density (number per site) of a lattice gas, and

$$f = \eta^{-2} - 1 \tag{4.6}$$

is analogous to (4.1) above. In terms of the standard transcription to the lattice gas,[16] we have

$$p/kT = \ln \Lambda, \tag{4.7}$$

$$\Phi/kT = 2\nu_2 \ln \eta + \ln \alpha, \tag{4.8}$$

$$\Psi/kT = 2\nu_2 \ln \eta + \ln \alpha - \ln \Lambda/\rho, \tag{4.9}$$

where p is the pressure, Φ the Gibbs free energy per particle, and Ψ the Helmholtz free energy per particle. As usual,

$$\Psi = U - TS,$$

$$\Phi = \Psi + p/\rho = \frac{\partial}{\partial \rho}(\rho\Psi)\Big|_T, \quad p = \rho^2 \frac{\partial \Psi}{\partial \rho}\Big|_T. \tag{4.10}$$

[42] N. M. Hugenholtz, Physica **23**, 533 (1957).
[43] B. D. Day, Rev. Mod. Phys. **39**, 719 (1967).
[44] R. Rajaraman and H. A. Bethe, Rev. Mod. Phys. **39**, 745 (1967).
[45] B. H. Brandow, Rev. Mod. Phys. **39**, 771 (1967).
[46] K. A. Brueckner, in *1965 Tokyo Summer Lectures in Theoretical Physics—Part 1, Many-Body Theory*, R. Kubo, Ed. (W. A. Benjamin, Inc., New York, 1966), p. 152.
[47] C. Bloch, in *Studies in Statistical Mechanics*, J. de Boer and G. E. Uhlenbeck, Eds. (John Wiley & Sons, Inc., New York, 1965), Vol. III.
[48] S. Katsura, Progr. Theoret. Phys. (Kyoto) **20**, 192 (1958) and references therein.
[49] R. A. Farrell, T. Morita, and P. H. E. Meijer, J. Chem. Phys. **45**, 349 (1966).
[50] G. S. Rushbrooke and H. I. Scoins, J. Math. Phys. **3**, 176 (1962); **4**, 998 (1963).

As we remarked before, Ψ is necessarily a convex function [Eq. (2.1)] of the volume, $1/\rho$. The coefficients β_k are tabulated by Rushbrooke and Scoins[50] and are polynomials in f. This fact allows us to re-express (4.4)–(4.5), and thus (4.7)–(4.9), as power series in f with coefficients which are polynomials in ρ. The expansion for Ψ is

$$\begin{aligned}\Psi\rho/kT = {} & [\rho \ln \rho + (1-\rho)\ln(1-\rho)] \\ & - 2\nu_2 \sum_{n=1}^{\infty} \frac{(2n-1)!\, f^n}{n!\,(n-1)!} \\ & \times \left[\sum_{r=0}^{n-1} \binom{n-1}{r} \frac{(-\rho)^{n+r+1}}{(n+r)(n+r+1)}\right] \\ & - \tfrac{1}{4}Af^4y^4 - \tfrac{1}{5}Bf^5y^5 - (\tfrac{1}{6}D + C)f^6y^6 \\ & - \tfrac{1}{5}Cf^6y^5 - (\tfrac{1}{7}F + E)f^7y^7 - \tfrac{1}{6}Ef^7y^6 \\ & - (\tfrac{9}{2}G + H + \tfrac{1}{8}K)f^8y^8 - (\tfrac{1}{7}H + G)f^8y^7 \\ & - \tfrac{1}{6}Gf^8y^6 - (5L + M + \tfrac{1}{9}N)f^9y^9 \\ & - (L + \tfrac{1}{8}M)f^9y^8 - \tfrac{1}{7}Lf^9y^7 + \cdots, \end{aligned} \tag{4.11}$$

where $y = \rho(1-\rho)$. The constants $\nu_2, A, \cdots, N$ are the Rushbrooke–Scoins parameters, which they do not tabulate completely, but do give all information necessary to obtain them. We list them in Table I. (We abbreviate the lattice structures, body-centered cubic, and simple cubic by B.C.C. and S.C., respectively.) It will be noted that, except for the coefficient of ν_2, Ψ_ρ is a function of y alone. The symmetry can be shown to be complete if we subtract $2\nu_2\rho \ln(\eta)$ from $\Psi\rho/kT$. As $\eta \propto \exp(J/kT)$ with J a constant, this changes Ψ by a constant only. However, it spoils the low-density behavior in that a finite number of powers of f now give a progressively better approximation in the low-density limit. Terms through f^4 are good to ρ^4, f^6 to ρ^5, f^8 to ρ^6, etc. The symmetry in ρ and $1-\rho$ is a reflection of spin-up, spin-down symmetry in the Ising model and cannot be expected in realistic gases.

The lattice-gas model has one advantage over the more realistic case in that the hard cores are automatically taken care of, whereas they still represent a complication in a realistic case.

TABLE I. Rushbrooke and Scoins parameters.

Lattice	B.C.C.	S.C.
ν_2	4	3
A	48	12
B	−480	−120
C	60	0
D	3408	924
E	288	108
F	−33264	−7476
G	162	0
H	−14238	−1890
K	378408	62940
L	896	56
M	181280	21616
N	−4033584	−535032

We need to solve for the coexistence curve (for fixed f). This can be done through the usual Gibbs double-tangent construction to Ψ. That is to say, we construct the convex hull of Ψ as a function of the volume, $1/\rho$. Alternatively, we can proceed analytically by means of the equations

$$\Delta p = p_{\text{liquid}} - p_{\text{gas}} = 0, \tag{4.12}$$

$$\Delta\Phi = \Phi_{\text{liquid}} - \Phi_{\text{gas}} = 0, \tag{4.13}$$

which are entirely equivalent to the double-tangent construction, and simply state that the pressure and the Gibbs free energy are constant throughout the two-phase region. It is convenient to our purposes to replace (4.13) by

$$\Delta(\Phi - 2p) = 0, \tag{4.14}$$

which is equivalent by (4.12). Now $\Phi - 2p$ is a function of ρ through y alone, and hence we must have

$$\rho_{\text{liquid}} + \rho_{\text{gas}} = 1. \tag{4.15}$$

Hence we may replace (4.13) by (4.15). If we eliminate ρ_{gas} from (4.12) by (4.15), from (4.8) and (4.14) and the symmetries of $\ln\alpha$ we derive in an obvious fashion that the equation for coexistence curve is

$$\ln\alpha = 0 \tag{4.16}$$

in Rushbrooke and Scoins[50] notation. We remark that very accurate results for the coexistence curve can be obtained through the use of Padé analysis of the low-temperature expansions of Sykes, Essam, and Gaunt[51] and the previous location of the critical point.[7] Therefore we have used these to calculate the densities which correspond to f values, which in turn correspond approximately to $T_c, 0.9T_c, 0.8T_c, 0.7T_c, 0.6T_c$, and $0.5T_c$. We have summed the series through the highly effective Padé approximant method.[52] In Table II we have tabulated the approximate values of f at each density. We also list the value of f from which the density was computed,[51] except for the critical point which was determined otherwise. We emphasize the early approximants formed from few terms (as are these) are most closely analogous with what is possible in the many-fermion case. We have tabulated only the results for the liquid side of the coexistence curve, since, by the aforementioned symmetry of $\ln\alpha$, the gaseous results are identical. We see that while the very earliest approximations are rather wide

[51] M. F. Sykes, J. W. Essam, and D. S. Gaunt, J. Math. Phys. 6, 283 (1965).
[52] G. A. Baker, Jr., Advan. Theoret. Phys. 1, 1 (1965).

TABLE II. Approximations to $f(\rho)$ on the coexistence curve.

ρ	f	zero of [0, 1]	zero of [1, 1]	zero of [2, 2]	zero of [5, 4]
$\frac{1}{2}$	0.877368	0.5000000	0.80000000	0.79168939	0.85699027
0.85505	1.0149103	0.62483647	1.0240838	0.99378839	1.0149738[a]
0.920873	1.1953897	0.72892111	1.2515262	1.1858001	1.1952015
0.9588476	1.4600746	0.85770570	1.5963165	1.4598220	1.4596850
0.98058240	1.8571429	1.0201078	2.1680313	1.8700941	1.8568898
0.99254822	2.5245098	1.2414576	3.3544837	2.5742320	2.5242016

[a] [4, 4] used here because of close pole and zero defect in [5, 4].

TABLE III. Approximations to Ψ/kT on the coexistence curve.

ρ	Ψ/kT	[0, 1]	[1, 1]	[2, 2]	[5, 4]
0.00745178	−5.96962732	−5.932571	−5.993124	−5.970856	−5.9696183
0.01941760	−5.07200178	−5.011036	−5.093456	−5.071996	−5.0719815
0.0411524	−4.399563	−4.310795	−4.416493	−4.396455	−4.3994217
0.079127	−3.85019	−3.726757	−3.857763	−3.839822	−3.8501198
0.14495	−3.3889	−3.217415	−3.377038	−3.360670	−3.388751[a]
$\frac{1}{2}$	...	−2.386294	−2.617064	−2.656686	−2.7393572
0.85505	−2.90174	−2.621070	−2.817055	−2.860930	−2.901746[a]
0.920873	−3.205995	−2.985377	−3.142835	−3.183741	−3.205644
0.9588476	−3.6350499	−3.468590	−3.586386	−3.623055	−3.634439
0.98058240	−4.216570114	−4.098859	−4.178916	−4.209376	−4.216261
0.99254822	−5.045952611	−4.973088	−5.018938	−5.040540	−5.045840

[a] [4, 4] used for consistency with Table II.

of the mark, the improvement is quite rapid and that, except near the critical point, the location of the coexistence curve is determined within about 0.02 % . Even the [2, 2] Padé approximant, which uses only 4 terms in the f series, gives about 2% in accuracy, except near the critical point where it is only 10% off.

In Table III we give the approximant values of Ψ/kT, evaluated at the corresponding approximate locations of the coexistence curve given in Table II. We also list, to as many figures as seem to us to be meaningful, the results obtained from the low-temperature expansion.[51] The relation is

$$\Psi/kT = -\nu_2 \ln (1+f) - \ln \Lambda/\rho, \qquad (4.17)$$

where Λ is that of Ref. 51. We obtain (except at $T = T_c$) at least four figure agreement, and in gaseous regions even better agreement. The major component of error in Table III stems from the approximate nature of the location of the coexistence curve. As is evident from Tables II and III, our results compare favorably with classical methods for dealing with this problem.[41] We have also computed the results for the simple cubic lattice, and they confirm those presented here for the body-centered cubic lattice; however, owing to its lower coordination numbers, the convergence is, as expected, not quite so rapid. We remark that the results of Kikuchi,[53] using the cluster-variation method, confirm that reasonable accuracy is possible from approximations based on the careful use of the properties of finite clusters, even quite small ones. He also finds that the free energy [actually he uses the pressure, which is closely related by (4.7) and (4.9)] is determined relatively more accurately than the location of the coexistence curve.

ACKNOWLEDGMENTS

The authors would like to thank Dr. V. J. Emery, Professor M. E. Fisher, and Professor G. S. Rushbrooke for discussions of some portions of this work.

[53] R. Kikuchi, Bull. Am. Phys. Soc. **12**, 485 (1967); Hughes Research Laboratory research reports 368 and 369.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Properties of "Quadratic" Canonical Commutation Relation Representations*

JOHN R. KLAUDER†
Bell Telephone Laboratories, Incorporated, Murray Hill, New Jersey
AND
L. STREIT
Department of Physics, Syracuse University, Syracuse, New York

(Received 28 February 1969)

A class of representations of the canonical commutation relations is studied, each of which is characterized by an expectation functional that is the exponential of a Euclidean-invariant quadratic form of the test functions. The underlying field operators are realized as the direct product of two Fock representations and the consequences of this realization are analyzed. Compatible Hamiltonians are constructed and an extensive study of the most general quadratic Hamiltonians is presented. In order to include thermodynamic examples, the analysis includes indefinite Hamiltonian spectra as well as the usual definite spectra. Finally, conditions are given for a theory to be local in the sense that all time derivatives of the field operator commute with one another at equal times but unequal spatial arguments.

1. INTRODUCTION

In an effort to shed light on the role in quantum theory of various representations of the canonical commutation relations (CCR), we have studied in some detail the properties of an important special class of representations. Included within this class are representations that pertain to a general quadratic Hamiltonian, and in particular to a relativistic free field, to a generalized free field, and to the extension of these examples to an equilibrium thermal ensemble at a nonzero temperature. Our original discussion is applicable to a rather general dynamical system having no special invariance properties. However, in view of the greater consequences that can be drawn, we treat in detail systems exhibiting Euclidean invariance, i.e., invariance under space translations and space rotations. Due to our inclusion of thermodynamic analogs, we do not restrict ourselves to Hamiltonians with positive spectra but instead make allowances for the occurrence of both signs of the energy.[1] Criteria are formulated for the spectrum of the Hamiltonian to have the energy–momentum relationship characteristic of a relativistic theory. In addition, the influence on the energy spectrum brought about by adopting the weak correspondence principle—a constraint on certain expectation values—is explored for the present models. Lastly, we ascertain the conditions on the CCR representation compatible with a Hamiltonian which behaves as the integral of a local density function in the sense that the mth time derivative of the field operator commutes with the nth time derivative of the field operator, for all m and n, when evaluated at equal times and unequal spatial arguments.

2. CHARACTERIZATION OF THE REPRESENTATIONS

The canonical commutation relations (CCR) may be given their most precise form with the aid of the unitary Weyl operators $U[f, g]$ which fulfill the combination law

$$U[f', g']U[f, g] = \exp\{\tfrac{1}{2}i[(f', g) - (g', f)]\} \times U[f' + f, g' + g], \quad (2.1)$$

where (f, g) represents the inner product of the two real functions f and g.[2] Minimal continuity arguments ensure that the Weyl operators have the form

$$U[f, g] = \exp\{i[\varphi(f) - \pi(g)]\}, \quad (2.2)$$

where $\varphi(f)$ and $\pi(g)$ are the self-adjoint smeared field and momentum operators, respectively, which, on an appropriate domain, fulfill the Heisenberg form of the commutation relations

$$[\varphi(f), \pi(g)] = i(f, g). \quad (2.3)$$

In a cyclic representation of the Weyl operators there exists a normalized vector $|0\rangle$ for which the vectors

$$|f, g\rangle \equiv U[f, g]\,|0\rangle \quad (2.4)$$

span the Hilbert space $\mathcal{H}$. Moreover, in a cyclic representation the representation of $U[f, g]$ is

* Work supported in part by a contract from the National Science Foundation.

† Work was done while at Syracuse University, Syracuse, New York.

[1] R. Haag, N. M. Hugenholtz, and M. Winnink, Commun. Math. Phys. **5**, 215 (1967).

[2] A number of studies of the canonical commutation relations exist in the literature. See, e.g., L. Gårding and A. S. Wightman, Proc. Natl. Acad. Sci. U.S. **40**, 617 (1954); A. S. Wightman and S. S. Schweber, Phys. Rev. **98**, 812 (1955); I. E. Segal, Trans. Am. Math. Soc. **88**, 12 (1958); J. S. Lew, Ph.D. thesis, Princeton University, 1960 (unpublished); H. Araki, J. Math. Phys. **1**, 492 (1960); J. R. Klauder and J. McKenna, *ibid.* **6** 68 (1965); L. Streit, Commun. Math. Phys. **4**, 22 (1967).

characterized,[3] apart from unitary equivalence, by the functional

$$\langle 0|\, U[f,g]\,|0\rangle = \langle 0|\exp\{i[\varphi(f)-\pi(g)]\}\,|0\rangle. \quad (2.5)$$

We shall study in some detail properties of those representations (and their associated dynamics) for which

$$\langle 0|\exp\{i[\varphi(f)-\pi(g)]\}\,|0\rangle = \exp\left\{-\tfrac{1}{4}\int[\alpha(k)\,|\tilde{f}(\mathbf{k})|^2+\beta(k)\,|\tilde{g}(\mathbf{k})|^2]\,d\mathbf{k}\right\}, \quad (2.6)$$

where $\tilde{f}(\mathbf{k})$ is the Fourier transform of the real smearing function $f(\mathbf{x})$ [and likewise for $\tilde{g}(\mathbf{k})$] and $\alpha(k)$ and $\beta(k)$ are nonnegative functions of $k=|\mathbf{k}|$ for which $\alpha(k)>0$, $\beta(k)>0$, and $\alpha(k)\beta(k)\geq 1$ for almost all k. In this notation (f,g) takes the form

$$(f,g)=\int f(\mathbf{x})g(\mathbf{x})\,d\mathbf{x}=\int \tilde{f}^*(\mathbf{k})\tilde{g}(\mathbf{k})\,d\mathbf{k}. \quad (2.7)$$

Due to their Gaussian form, we term such representations "quadratic" CCR representations.[4] As we shall see below, these representations, which are evidently characterized by the functions α and β, fall into two categories: The representation is *irreducible* if and only if $\alpha(k)\beta(k)=1$ for almost all k; the representation is *reducible* if $\alpha(k)\beta(k)>1$ holds for some k set of nonzero measure. It may be shown that two representations $U[f,g]$ and $U'[f,g]$ are unitarily equivalent, i.e., there exists a unitary transformation V such that

$$VU[f,g]V^{-1}=U'[f,g], \quad (2.8)$$

provided that $\alpha(k)=\alpha'(k)$ and $\beta(k)=\beta'(k)$ for almost all k. In other words, distinct function pairs $\alpha(k)$, $\beta(k)$ label unitarily inequivalent "quadratic" CCR representations.[5]

The class of allowed argument functions f and g depends on the specific choice of α and β. For concreteness, it suffices to consider $\tilde{f}(\mathbf{k})\in L^2(R^3,\alpha)$, $\tilde{g}(\mathbf{k})\in L^2(R^3,\beta)$, where $\alpha\,d\mathbf{k}$ and $\beta\,d\mathbf{k}$ are the integration measures, respectively, and we have assumed a three-dimensional configuration space. The relation $\alpha\beta\geq 1$ coupled with Schwarz's inequality ensures that (f,g) will be well defined. Alternatively, we may take both $\tilde{f}(\mathbf{k})$ and $\tilde{g}(\mathbf{k})$ as elements of $L^2(R^3,[\alpha^2+\beta^2]^{\frac{1}{2}})$, which is evidently dense in the spaces $L^2(R^3,\alpha)$ and $L^2(R^3,\beta)$. If $[\alpha^2+\beta^2]^{\frac{1}{2}}<p(k)$ where p is some polynomial, then yet a further choice is to take $\tilde{f}(\mathbf{k})$ and $\tilde{g}(\mathbf{k})$ as elements of $\mathcal{S}(R^3)$, Schwartz's space of infinitely differentiable test functions of rapid decrease.[6] In the present case it is evident that the elements of $\mathcal{S}(R^3)$ are dense in $L^2(R^3,[\alpha^2+\beta^2]^{\frac{1}{2}})$. Clearly there is considerable flexibility in the matter for a given $\alpha(k)$ and $\beta(k)$, but there seems to be no universal set of test functions that apply to all "quadratic" CCR representations irrespective of the choice of α and β.[7]

A number of specific physical systems are characterized by having "quadratic" CCR representations. Among these we note the free relativistic scalar field of mass m for which

$$\alpha(k)=\beta^{-1}(k)=(k^2+m^2)^{-\frac{1}{2}}\equiv\omega(k)^{-1} \quad (2.9)$$

and the generalized free field[8] for which

$$\alpha(k)=\int\omega(k)^{-1}\rho(m^2)\,dm^2, \quad (2.10a)$$

$$\beta(k)=\int\omega(k)\rho(m^2)\,dm^2, \quad (2.10b)$$

where $\rho(m^2)\geq 0$ is the mass distribution so normalized that

$$\int\rho(m^2)\,dm^2=1. \quad (2.11)$$

In the latter case, if ρ has support other than at a single point, it follows that $\alpha(k)\beta(k)>1$ for all k and the corresponding representation is reducible. In addition, a free scalar field of mass m in thermal equilibrium at temperature T has a "quadratic" CCR representation characterized by

$$\alpha(k)=\omega(k)^{-1}[1+n(k)], \quad (2.12a)$$

$$\beta(k)=\omega(k)[1+n(k)], \quad (2.12b)$$

where

$$n(k)\equiv\{\exp[\omega(k)/\kappa T]-1\}^{-1} \quad (2.13)$$

and κ denotes Boltzmann's constant.[9] Here $\alpha\beta>1$ for all k if $T>0$, and the corresponding representation is reducible. In a like manner, a generalized free field in thermal equilibrium at temperature T is characterized by

$$\alpha(k)=\int\omega(k)^{-1}[1+n(k)]\rho(m^2)\,dm^2, \quad (2.14a)$$

$$\beta(k)=\int\omega(k)[1+n(k)]\rho(m^2)\,dm^2. \quad (2.14b)$$

[3] M. A. Naimark, *Normed Rings* (Noordhoff, Groningen, The Netherlands, 1959), p. 242.

[4] Such CCR representations have also been studied by H. Araki and E. J. Woods, J. Math. Phys. **4**, 637 (1965); D. W. Robinson, Commun. Math. Phys. **1**, 159 (1965); G. F. Dell'Antonio, *ibid.* **9**, 81 (1968); J. Manuceau and A. Verbeure (to be published).

[5] See, e.g., J. R. Klauder, "Coherence, Correlation and Quantum Field Theory," Brandeis Summer School, 1967.

[6] L. Schwartz, *Theorie des distributions* (Hermann & Cie., Paris, 1957), Vol. II.

[7] Regarding the dependence of test function spaces on the given CCR representation, see L. Streit, Commun. Math. Phys. **4**, 22 (1967).

[8] O. W. Greenberg, Ann. Phys. (N.Y.) **16**, 158 (1961).

[9] This result is a simple generalization of the answer obtained by H. Araki and E. J. Woods [J. Math. Phys. **4**, 637 (1963)] for the zero-mass case.

To indicate that systems exhibiting interaction are not excluded by the restriction to "quadratic" CCR representations, we cite the case of the exactly soluble rotationally symmetric models[10] for which $\alpha(k) = \xi/m$, $\beta(k) = m$, with $\alpha\beta = \xi > 1$. Our discussion will indicate further classes of systems for which such representations apply.

3. REALIZATION AND PROPERTIES OF THE REPRESENTATIONS

Irreducible Case

If we denote the special irreducible representation for which $\alpha(k) = \beta(k) = 1$ by the subscript F (for Fock), then the field operators for the general irreducible "quadratic" CCR representation may be expressed in the form

$$\varphi(f) = \varphi_{\mathrm{F}}(\alpha^{\frac{1}{2}}f), \tag{3.1a}$$

$$\pi(g) = \pi_{\mathrm{F}}(\beta^{\frac{1}{2}}g), \tag{3.1b}$$

which, since $\alpha\beta = 1$, is a canonical transformation that preserves the CCR. Here we have used the notation $\alpha^{\frac{1}{2}}f$ and $\beta^{\frac{1}{2}}g$ to correspond to those elements which in momentum space are $\alpha^{\frac{1}{2}}(k)\tilde{f}(\mathbf{k})$ and $\beta^{\frac{1}{2}}(k)\tilde{g}(\mathbf{k})$, respectively. According to the remarks made above, the transformation from $\varphi_{\mathrm{F}}(f)$ to $\varphi_{\mathrm{F}}(\alpha^{\frac{1}{2}}f)$ cannot be carried out by a unitary transformation since distinct α (recall here $\beta = \alpha^{-1}$) label unitarily inequivalent representations. Nonetheless, Eq. (3.1) ensures that the properties of φ are easily determined from those of φ_{F}, etc.

The special Fock fields are characterized by the formal properties that the momentum space field $\tilde{\varphi}(\mathbf{k})$ and its conjugate momentum $\tilde{\pi}(\mathbf{k})$ admit a decomposition into creation and annihilation operators $a^{\dagger}(\mathbf{k})$ and $a(\mathbf{k})$, respectively, in the simple fashion:

$$\tilde{\varphi}_{\mathrm{F}}(\mathbf{k}) \equiv 2^{-\frac{1}{2}}[a(\mathbf{k}) + a^{\dagger}(-\mathbf{k})], \tag{3.2a}$$

$$\tilde{\pi}_{\mathrm{F}}(\mathbf{k}) \equiv -i(2)^{-\frac{1}{2}}[a(\mathbf{k}) - a^{\dagger}(-\mathbf{k})]. \tag{3.2b}$$

As is customary,

$$[a(\mathbf{k}), a^{\dagger}(\mathbf{k}')] = \delta(\mathbf{k} - \mathbf{k}'); \tag{3.3}$$

all other commutators are vanishing. The usual no-particle state $|0\rangle$ is invariant against spatial rotations and translations, and for all $\mathbf{k}$ fulfills

$$a(\mathbf{k})\,|0\rangle = 0. \tag{3.4}$$

All states in the Hilbert space $\mathcal{H}_{\mathrm{F}}$ are determined from normalizable linear combinations of the Fock states

$$|\mathbf{k}_1, \cdots, \mathbf{k}_n\rangle \equiv (n!)^{-\frac{1}{2}}a^{\dagger}(\mathbf{k}_1)\cdots a^{\dagger}(\mathbf{k}_n)\,|0\rangle \tag{3.5}$$

for all $\mathbf{k}_j$ and all $n \geq 0$. On combining this fact with (3.2) and (3.3), it is clear that $\mathcal{H}_{\mathrm{F}}$ is spanned by vectors of the form

$$\tilde{\varphi}_{\mathrm{F}}(\mathbf{k}_1)\cdots\tilde{\varphi}_{\mathrm{F}}(\mathbf{k}_n)\,|0\rangle \tag{3.6a}$$

or by those of the form

$$\tilde{\pi}_{\mathrm{F}}(\mathbf{k}_1)\cdots\tilde{\pi}_{\mathrm{F}}(\mathbf{k}_n)\,|0\rangle \tag{3.6b}$$

for all $\mathbf{k}_j$ and all n. Thus $|0\rangle$ is a cyclic vector for the field φ or the momentum π. This is frequently stated from the generating function point of view, namely,

$$\mathcal{H}_{\mathrm{F}} = \overline{\{\exp[i\varphi(f)]\}\,|0\rangle} = \overline{\{\exp[-i\pi(g)]\}\,|0\rangle}, \tag{3.7}$$

where the overbar denotes the closed linear space formed by taking all normalizable linear combinations of the indicated vectors.

Another familiar fact we shall employ deals with the completeness of the Fock operators, i.e., that all operators on $\mathcal{H}_{\mathrm{F}}$ can be built from the φ_{F} and π_{F}. The precise rendition of this fact is frequently stated in terms of the commutant $\{A\}'$ of a family of operators A which is defined as the set of bounded operators each of which commutes with the operators A. Thus, the irreducibility of φ_{F} and π_{F} may be stated as

$$\{U_{\mathrm{F}}[f, g]\}' = \{I\}, \tag{3.8a}$$

where $\{I\}$ is composed solely of multiples of the identity. Additionally, therefore, the double commutant

$$\{U_{\mathrm{F}}[f, g]\}'' = \mathfrak{B}(\mathcal{H}_{\mathrm{F}}), \tag{3.8b}$$

where $\mathfrak{B}(\mathcal{H}_{\mathrm{F}})$ denotes the set of all bounded operators on the Hilbert space $\mathcal{H}_{\mathrm{F}}$.

Reducible Case

For the reducible representations, it is convenient to introduce

$$\gamma(k) \equiv \frac{\beta(k)\alpha(k) - 1}{\alpha(k)} = \beta(k) - \frac{1}{\alpha(k)}, \tag{3.9}$$

which, by hypothesis, is positive for a $\mathbf{k}$ set Γ' of nonzero measure. [The complementary set Γ is defined as the set of $\mathbf{k}$ for which $\gamma(k) = 0$.] With this we may write the basic functional (2.6) for the "quadratic" CCR representations as

$$\langle 0|\exp\{i[\varphi(f) - \pi(g)]\}\,|0\rangle = \exp\left\{-\tfrac{1}{4}\int[\alpha(k)\,|\tilde{f}(\mathbf{k})|^2 + \alpha^{-1}(k)\,|\tilde{g}(\mathbf{k})|^2]\,d\mathbf{k}\right\} \times \exp\left\{-\tfrac{1}{4}\int[\gamma(k)\,|\tilde{g}(\mathbf{k})|^2]\,d\mathbf{k}\right\}. \tag{3.10}$$

In this form it is rather apparent that φ and π may be

[10] J. R. Klauder, J. Math. Phys. 6, 1666 (1965).

decomposed into two Fock fields as given by

$$\varphi(f) = \varphi_F(\alpha^{\frac{1}{2}}f) \otimes 1, \tag{3.11a}$$

$$\pi(g) = \pi_F(\alpha^{-\frac{1}{2}}g) \otimes 1 + 1 \otimes \pi_F(\gamma^{\frac{1}{2}}g). \tag{3.11b}$$

The first entry in the direct-operator product corresponds to the "first" field while the second entry corresponds to the "second" field. Clearly, the Heisenberg form of the CCR is fulfilled by the "first" field; the second term in $\pi(g)$ commutes with $\varphi(f)$. Whether or not these two fields should be called "independent" can only be answered after the dynamics have been formulated. There are cases where the pair of fields have an independent history and other cases where they become mixed together. In any case, the field operators and the associated dynamical evolution are reduced to computations involving two Fock-like representations, which evidently can be represented in a Hilbert space $\mathcal{H} \subseteq \mathcal{H}_F \otimes \mathcal{H}_F$. Here, equality holds if and only if $\gamma > 0$ for almost all $\mathbf{k}$, i.e., the set Γ has zero measure. If Γ has positive measure, then we may set $\mathcal{H} = \mathcal{H}_F \otimes \mathcal{H}_{F,\Gamma}$, where $\mathcal{H}_{F,\Gamma}$ denotes the Hilbert space formally composed of normalizable linear combinations of the vectors (3.5) restricted so that $\mathbf{k}_j \in \Gamma'$. For simplicity we shall assume for the most part that $\gamma > 0$ for almost all $\mathbf{k}$ so that $\mathcal{H}_{F,\Gamma} = \mathcal{H}_F$.

The reducibility of the field operators φ and π is clear from (3.11) since it is evident, for example, that the operator $1 \otimes \pi_F(\gamma^{\frac{1}{2}}g)$ commutes with both φ and π and differs from the unit operator. To characterize such commuting operators let us define the "dual" Weyl operators

$$U'[r, s] \equiv \exp\{i[\varphi'(r) - \pi'(s)]\}, \tag{3.12}$$

where r and s denote test functions and where

$$\varphi'(r) \equiv -\varphi_F(\alpha^{\frac{1}{2}}r) \otimes 1 + 1 \otimes \varphi_F(\gamma^{-\frac{1}{2}}r), \tag{3.13a}$$

$$\pi'(s) \equiv 1 \otimes \pi_F(\gamma^{\frac{1}{2}}s). \tag{3.13b}$$

Here, $\gamma^{-\frac{1}{2}}$ is defined only on Γ', the set for which $\gamma > 0$. By construction, the primed fields commute with the unprimed ones and, moreover, they generate all such fields so that

$$\{U[f, g]\}' = \{U'[r, s]\}'', \tag{3.14a}$$

$$\{U[f, g]\}'' = \{U'[r, s]\}'. \tag{3.14b}$$

We note in addition the relations

$$\{e^{i\varphi(f)}\}' = \{e^{i\varphi_F(f)}\}' \otimes \mathcal{B}(\mathcal{H}_F), \tag{3.15a}$$

$$\{e^{i\varphi(f)}\}'' = \{e^{i\varphi_F(f)}\}'' \otimes 1. \tag{3.15b}$$

The latter relation implies that, unlike the irreducible case, the field operators $\varphi(f)$ are no longer cyclic. Indeed, Eq. (3.15b) leads to

$$\overline{\exp[i\varphi(f)]\,|0\rangle} = \mathcal{H}_F \otimes \Omega_F, \tag{3.16}$$

which is heuristically evident from (3.11a). However, since π involves the "second" field,

$$\overline{U[f, g]\,|0\rangle} = \mathcal{H}_F \otimes \mathcal{H}_F = \mathcal{H}; \tag{3.17a}$$

and, in like fashion, a similar argument shows that

$$\overline{U'[r, s]\,|0\rangle} = \mathcal{H}_F \otimes \mathcal{H}_F = \mathcal{H}. \tag{3.17b}$$

We note, in contrast to the irreducible case, if $A\,|0\rangle = 0$ and $A \in \{U[f, g]\}''$, then $A = 0$. This follows because the cyclic vector of a von Neumann algebra—$\{U'[r, s]\}''$ in our case—is separating for its commutant.[11] On the other hand, and again in contrast to the irreducible case, there do exist nonzero annihilation operators $A \in \{e^{i\varphi(f)}\}'$. Specifically, if $A_F \in \mathcal{B}(\mathcal{H}_F)$ annihilates the no-particle state in $\mathcal{H}_F$, then $A = 1 \otimes A_F \in \{e^{i\varphi(f)}\}'$ annihilates $|0\rangle$.

As is common in a canonical approach, we shall ask that the Hamiltonian H connect the field and momentum via the usual relation

$$i[H, \varphi] = \pi. \tag{3.18}$$

From the foregoing commutation relations it may be seen that

$$H_{00} = \int b^\dagger(\mathbf{k}) b(\mathbf{k})\, d\mathbf{k}, \tag{3.19}$$

where

$$b(\mathbf{k}) \equiv \alpha^{-\frac{1}{2}}(k) a_1(\mathbf{k}) + \gamma^{\frac{1}{2}}(k) a_2(\mathbf{k}) \tag{3.20}$$

already fulfills the requirement (3.18). Here

$$a_1(\mathbf{k}) \equiv a(\mathbf{k}) \otimes 1, \tag{3.21a}$$

$$a_2(\mathbf{k}) \equiv 1 \otimes a(\mathbf{k}) \tag{3.21b}$$

denote annihilation operators for the "first" and "second" fields, respectively. In consequence, $H - H_{00} \equiv \mathfrak{U}$ commutes with φ and thus $\mathfrak{U}$ is a function of $\{e^{i\varphi(f)}\}'$.

The no-particle state $|0\rangle$ fulfills the relations

$$a_1(\mathbf{k})\,|0\rangle = a_2(\mathbf{k})\,|0\rangle = 0 \tag{3.22}$$

for all $\mathbf{k}$. As a consequence, the state $|0\rangle$ (and no other state) is invariant under spatial rotations and translations for which the infinitesimal generators read

$$\mathfrak{J} = \sum_{l=1,2} \int a_l^\dagger(\mathbf{k}) \left(i \frac{\partial}{\partial \mathbf{k}} \times \mathbf{k} \right) a_l(\mathbf{k})\, d\mathbf{k}, \tag{3.23a}$$

$$\mathfrak{P} = \sum_{l=1,2} \int a_l^\dagger(\mathbf{k}) \mathbf{k} a_l(\mathbf{k})\, d\mathbf{k}, \tag{3.23b}$$

[11] J. Dixmier, *Les algèbres d'opérateurs dans l'espace hilbertien* (Gauthier-Villars, Paris, 1957), Chap. I, Sec. 1, Proposition 5 and corollary.

respectively. In a Euclidean-invariant theory the Hamiltonian H commutes with both $\mathfrak{I}$ and $\mathfrak{T}$. Thus either $|0\rangle$ is an eigenstate of H (which we assume adjusted to eigenvalue zero) or it is taken into a nonnormalizable vector. It is the essence of Haag's theorem[12] that for the irreducible Fock representation only the free field Hamiltonian can annihilate $|0\rangle$, while every other proposed Euclidean-invariant Hamiltonian carries $|0\rangle$ into a nonnormalizable vector in virtue of vacuum polarization. However, for a reducible "quadratic" representation of the type considered here, such a "no-go" theorem does not apply. We note first that H_{00}, as the analog of a free-field Hamiltonian, annihilates the no-particle state $|0\rangle$. Secondly, we note that $\mathfrak{U} = H - H_{00}$ can be expressed in terms of $\{e^{i\varphi(f)}\}'$, which contains annihilation operators for $|0\rangle$ unlike the irreducible case. It is by exploiting such operators in the reducible representations that nontrivial Euclidean-invariant canonical theories can be formulated that circumvent Haag's theorem. While some such models have been formulated, we content ourselves here with a discussion of the single-particle sector of Hilbert space for which a simplified or reduced Hamiltonian is sufficient. Such an analysis is, in any case, a necessary preliminary to the analysis of the dynamics in higher-particle sectors.

4. PROPERTIES OF "FREE" HAMILTONIANS

Although the Hamiltonian H_{00} in Eq. (3.19) is positive, leads to $\dot{\varphi} = \pi$, and annihilates the vacuum, it is deficient in one respect to serve as a model for a free Hamiltonian. Since H_{00} only "tests" the presence of one form of excitation, there will be a multitude of distinct states having energy eigenvalue zero. Specifically, the creation operator

$$c^\dagger(\mathbf{q}) = -\alpha^{\frac{1}{2}}(q)a_1^\dagger(\mathbf{q}) + \gamma^{-\frac{1}{2}}(q)a_2^\dagger(\mathbf{q}) \tag{4.1}$$

commutes with both $b(\mathbf{k})$ and $b^\dagger(\mathbf{k})$ for all $\mathbf{k}$, and thus the Fock states

$$|\mathbf{q}_1, \cdots, \mathbf{q}_n\rangle_0 \equiv (n!)^{-\frac{1}{2}}c^\dagger(\mathbf{q}_1)\cdots c^\dagger(\mathbf{q}_n)\,|0\rangle \tag{4.2}$$

each fulfill

$$H_{00}\,|\mathbf{q}_1, \cdots, \mathbf{q}_n\rangle_0 = 0 \tag{4.3}$$

for all n and all $\mathbf{q}_j$ values (at least $\mathbf{q}_j \in \Gamma'$). Hence the entire infinite-dimensional subspace of normalizable vectors spanned by these Fock states is characterized by the fact that H_{00} has eigenvalue zero.

[12] See, for example, A. S. Wightman, *Lecture Notes at the French Summer School of Theoretical Physics, Cargese, Corsica, July, 1964*; L. Streit, "A Generalization of Haag's Theorem," Nuovo Cimento (to be published).

The most general quadratic Hamiltonian that fulfills (3.18) and retains Euclidean invariance also has the potential to lift this degeneracy. The form of this most general Hamiltonian reads

$$\begin{aligned} H_0 &= H_{00} + \int r(k)a_2^\dagger(\mathbf{k})a_2(\mathbf{k})\,d\mathbf{k} \\ &= \int [b^\dagger(\mathbf{k})b(\mathbf{k}) + r(k)a_2^\dagger(\mathbf{k})a_2(\mathbf{k})]\,d\mathbf{k}. \end{aligned} \tag{4.4}$$

Here $r(k)$ can be a rather general real function of k and still ensure Hermiticity of H_0. However, for generality we do not require that H_0 be positive; instead we permit $r(k)$ to assume both positive and negative values. Since

$$[\varphi(\mathbf{x}), a_2(\mathbf{k})] = [\varphi(\mathbf{x}), a_2^\dagger(\mathbf{k})] = 0, \tag{4.5}$$

it is evident that

$$i[H_0, \varphi(\mathbf{x})] = \pi(\mathbf{x}), \tag{4.6}$$

as desired.

Since H_0 is quadratic at each point $\mathbf{k}$, it is plausible that independent normal modes can be introduced which diagonalize H_0. The energy roots that follow from such a diagonalization are given by

$$E_\pm(k) = \tfrac{1}{2}\{\beta + r \pm [(\beta + r)^2 - 4r/\alpha]^{\frac{1}{2}}\}. \tag{4.7}$$

The radical term has the equivalent forms

$$\begin{aligned} Q &= [(\beta + r)^2 - 4r/\alpha]^{\frac{1}{2}} \\ &= [(\beta - r)^2 + 4r(\alpha\beta - 1)/\alpha]^{\frac{1}{2}}, \end{aligned} \tag{4.8}$$

which, since $\alpha\beta \geq 1$, shows Q to be real (and nonnegative by definition) regardless of r. Evidently, $E_+(k) > 0$ for almost all $\mathbf{k}$, while $E_-(k)$ has the sign of $r(k)$, i.e.,

$$E_-(k) \gtreqless 0, \quad \text{when } r(k) \gtreqless 0. \tag{4.9}$$

If $\alpha\beta > 1$, then $E_+ - E_- = Q > 0$; only if $\alpha\beta = 1$ and $r = \beta$ does $Q = 0$ leading to $E_+ = E_-$. In any term where $E_+ - E_-$ appears as a divisor, we shall implicitly assume the latter condition does not hold.

Let us also introduce the "spectral weights"

$$\rho_\pm = \pm E_\pm(1 - \alpha E_\pm)/(E_+ - E_-), \tag{4.10}$$

which satisfy the identity

$$\rho_+ + \rho_- = 1. \tag{4.11}$$

Unlike the usual case, one of these "weights" may assume negative values. In fact, as we shall indirectly show below,

$$\rho_+ > 0, \quad \text{when} \quad E_+ > 0, \tag{4.12a}$$

$$\rho_- \gtreqless 0, \quad \text{when} \quad E_- \gtreqless 0. \tag{4.12b}$$

Direct substitution of the above relations shows that

$$\alpha = \rho_+/E_+ + \rho_-/E_-, \tag{4.13a}$$
$$\beta = E_+\rho_+ + E_-\rho_-, \tag{4.13b}$$
$$r = E_-\rho_+ + E_+\rho_- = E_+E_-\alpha. \tag{4.13c}$$

Note that $\beta + r = E_+ + E_-$. Evidently the three functions E_+, E_-, and ρ_+ are a substitute set for α, β, and r.

We introduce two destruction operators $a_\pm(\mathbf{k})$ *via* suitable linear combinations

$$a_\pm(\mathbf{k}) = \alpha^{-\frac{1}{2}}[\pm(\rho_\pm/E_\pm)^{\frac{1}{2}}a_1(\mathbf{k}) + (\rho_\mp/E_\mp)^{\frac{1}{2}}a_2(\mathbf{k})] \tag{4.14}$$

which are independent, i.e.,

$$[a_-(\mathbf{k}), a_+(\mathbf{k}')] = [a_-(\mathbf{k}), a_+^\dagger(\mathbf{k}')] = 0 \tag{4.15a}$$

and are conventionally normalized in the sense that

$$[a_\pm(\mathbf{k}), a_\pm^\dagger(\mathbf{k}')] = \delta(\mathbf{k} - \mathbf{k}'). \tag{4.15b}$$

In terms of these operators, the Hamiltonian is resolved into independent normal modes according to

$$H_0 = \int [E_+(k)a_+^\dagger(\mathbf{k})a_+(\mathbf{k}) + E_-(k)a_-^\dagger(\mathbf{k})a_-(\mathbf{k})]\, d\mathbf{k}. \tag{4.16}$$

Finally, we note that the Hilbert space $\mathcal{H}$ may also be written in the related form

$$\mathcal{H} = \mathcal{H}_+ \otimes \mathcal{H}_-, \tag{4.17}$$

where $\mathcal{H}_\pm$ is the space spanned by repeated action of the creation operator $a_\pm^\dagger$ on the no-particle state $|0\rangle$.

Armed with the relation (4.16) for H_0, it is not difficult to find an expression for the two-point function

$$\langle 0|\, \varphi(\mathbf{x})e^{-iH_0t}\varphi(\mathbf{y})\, |0\rangle. \tag{4.18}$$

By noting that

$$\begin{aligned}\varphi(\mathbf{y})\, |0\rangle &= \frac{1}{(2)^{\frac{1}{2}}(2\pi)^{\frac{3}{2}}}\int e^{-i\mathbf{k}\cdot\mathbf{y}}\alpha^{\frac{1}{2}}(k)a_1^\dagger(\mathbf{k})\, d\mathbf{k}\, |0\rangle \\ &= \frac{1}{(2)^{\frac{1}{2}}}\frac{1}{(2\pi)^{\frac{3}{2}}}\int e^{-i\mathbf{k}\cdot\mathbf{y}}\left[\left(\frac{\rho_+}{E_+}\right)^{\frac{1}{2}}a_+^\dagger(\mathbf{k})\right. \\ &\quad \left. - \left(\frac{\rho_-}{E_-}\right)^{\frac{1}{2}}a_-^\dagger(\mathbf{k})\right] d\mathbf{k}\, |0\rangle,\end{aligned} \tag{4.19}$$

as follows from (4.14), we can readily deduce that

$$\begin{aligned}&\langle 0|\, \varphi(\mathbf{x})e^{-iH_0t}\varphi(\mathbf{y})\, |0\rangle \\ &\quad = \frac{1}{2}\frac{1}{(2\pi)^3}\int e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\left[\frac{\rho_+}{E_+}(k)e^{-iE_+(k)t}\right. \\ &\qquad \left. + \frac{\rho_-}{E_-}(k)e^{-iE_-(k)t}\right] d\mathbf{k},\end{aligned} \tag{4.20}$$

owing to the independent time evolution of the "+" and "−" modes. If we let

$$|\mathbf{k}, \pm\rangle \equiv a_\pm^\dagger(\mathbf{k})\, |0\rangle \tag{4.21}$$

denote the single-particle eigenstates of H_0, then evidently

$$\rho_\pm(k)/E_\pm(k) = 2(2\pi)^3\, |\langle 0|\, \varphi(0)\, |\mathbf{k}, \pm\rangle|^2, \tag{4.22}$$

which demonstrates that the sign of ρ is linked to that of E. On comparing the relation

$$\begin{aligned}&\langle 0|\, \varphi(\mathbf{x})\varphi(\mathbf{y})\, |0\rangle \\ &\quad = \frac{1}{2}\frac{1}{(2\pi)^3}\int e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\left[\frac{\rho_+}{E_+}(k) + \frac{\rho_-}{E_-}(k)\right] d\mathbf{k}\end{aligned} \tag{4.23}$$

with Eq. (2.6) expanded to the same order in φ, i.e.,

$$\langle 0|\left\{\int \varphi(\mathbf{x})f(\mathbf{x})\, d\mathbf{x}\right\}^2 |0\rangle = \tfrac{1}{2}\int |\tilde{f}(\mathbf{k})|^2\, \alpha(k)\, d\mathbf{k}, \tag{4.24}$$

we are led to the verification of (4.13a). In like manner two derivatives with respect to t lead to the relation

$$\begin{aligned}&\langle 0|\, \varphi(\mathbf{x})H_0^2\varphi(\mathbf{y})\, |0\rangle \\ &\quad = \langle 0|\, [\varphi(\mathbf{x}), H_0][H_0, \varphi(\mathbf{y})]\, |0\rangle \\ &\quad = \langle 0|\, \pi(\mathbf{x})\pi(\mathbf{y})\, |0\rangle \\ &\quad = \frac{1}{2}\frac{1}{(2\pi)^3}\int e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}[E_+(k)\rho_+(k) + E_-(k)\rho_-(k)]\, d\mathbf{k}.\end{aligned} \tag{4.25}$$

The expansion of (2.6) to the same order in π leads to

$$\langle 0|\left\{\int \pi(\mathbf{x})g(\mathbf{x})\, d\mathbf{x}\right\}^2 |0\rangle = \tfrac{1}{2}\int |\tilde{g}(\mathbf{k})|^2\, \beta(k)\, d\mathbf{k}, \tag{4.26}$$

which, on comparison with (4.25), establishes the validity of (4.13b).

Lastly, we note for reference the relation

$$\begin{aligned}\langle 0|\, \varphi(\mathbf{x})H_0^3\varphi(\mathbf{y})\, |0\rangle &= \langle 0|\, \pi(\mathbf{x})H_0\pi(\mathbf{y})\, |0\rangle \\ &= \frac{1}{2}\frac{1}{(2\pi)^3}\int e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\Omega^2(k)\, d\mathbf{k},\end{aligned} \tag{4.27}$$

where we have introduced the abbreviation

$$\Omega^2(k) \equiv E_+^2(k)\rho_+(k) + E_-^2(k)\rho_-(k). \tag{4.28}$$

Relativistic Covariance of One-Particle States

One natural condition that might be imposed on the one-particle states is the relativistic energy–momentum relation

$$E_\pm(k) = (k^2 + \mu_\pm^2)^{\frac{1}{2}} \equiv \omega_\pm, \tag{4.29}$$

where $\mu_+ > \mu_- \geq 0$, in the case that $E_- \geq 0$. These relations do not uniquely fix the parameters α, β, and r since no requirement has been imposed on ρ_+ (or

$\rho_- = 1 - \rho_+$). From the relations

$$\begin{aligned}\alpha &= \omega_+^{-1}\rho_+ + \omega_-^{-1}\rho_- \\ &= \omega_+^{-1} + \rho_-(\omega_+ - \omega_-)(\omega_+\omega_-)^{-1} \\ &= \omega_-^{-1} - \rho_+(\omega_+ - \omega_-)(\omega_+\omega_-)^{-1}, \end{aligned} \tag{4.30}$$

it is apparent that a suitable ρ_+ exists which satisfies the bounds $0 < \rho_+ < 1$ whenever the condition

$$\omega_-^{-1}(k) > \alpha(k) > \omega_+^{-1}(k) \tag{4.31}$$

is satisfied. Given such a condition on α, Eq. (4.13a) fixes ρ_+, which then, through (4.13b) and (4.13c), fixes β and r uniquely. In particular, we may put

$$\beta = \omega_+\rho_+ + \omega_-\rho_- = \omega_+ + \omega_- - \omega_-\omega_+\alpha, \tag{4.32a}$$

$$r = \omega_-\omega_+\alpha. \tag{4.32b}$$

For very large k values, $\omega_+ \simeq \omega_- \simeq k$, which leads to $\alpha \simeq k^{-1}$ and $\beta \simeq k \simeq r$. Thus, for very large k, $\alpha\beta \to 1$, which, roughly speaking, means that these modes tend toward irreducibility.

In the indefinite relativistic energy case for which

$$E_\pm(k) = \pm(k^2 + \mu_\pm^2)^{\frac{1}{2}} = \pm\omega_\pm \tag{4.33}$$

(and thus $\rho_- < 0$), a solution to the relation (4.30) exists so long as

$$\alpha(k) > \omega_+^{-1}(k). \tag{4.34}$$

Equations (4.32) still determine β and r. For very large k, $\omega_\pm \simeq \pm k$ so that $\beta \simeq k^2\alpha$ and $r \simeq -k^2\alpha$. Hence $\alpha\beta \simeq k^2\alpha^2$, which tends toward unity, and thus irreducibility for such modes, only if $k\alpha \to 1$ for large k.

It is worth making the qualitative remark that the high k behavior of the product $\alpha\beta$ is loosely connected with the degree of locality attainable in the interaction term $\mathfrak{U} = H - H_0$. Unfortunately, no fully relativistic examples are known for which $\mathfrak{U} \neq 0$.

In the context of the free theory where $\mathfrak{U} = 0$, it is straightforward to embed time translations and Euclidean transformations in a unitary representation $U(a, \lambda)$ of the Poincaré group $\{a, \lambda\}$. Here $U(a, \lambda)$ factorizes as

$$U(a, \lambda) = U_+(a, \lambda) \otimes U_-(a, \lambda) \tag{4.35}$$

with $U_\pm \in \mathfrak{B}(\mathcal{K}_\pm)$ the usual representations generated by multiparticle states of mass $\mu_\pm$ bosons.[13] (However, all momenta lie in the backward cone for U_- if $E_- < 0$.) This product structure reflects itself in the additive form of the ten generators. The Hamiltonian has already been given in Eq. (4.16). The space rotation and translation generators (3.24) may also be given a compatible form as follows:

$$\mathfrak{J} = \sum_{\lambda=+,-} \int a_\lambda^\dagger(\mathbf{k}) \left(i\frac{\partial}{\partial \mathbf{k}} \times \mathbf{k} \right) a_\lambda(\mathbf{k})\, d\mathbf{k}, \tag{4.36a}$$

$$\mathfrak{P} = \sum_{\lambda=+,-} \int a_\lambda^\dagger(\mathbf{k}) \mathbf{k} a_\lambda(\mathbf{k})\, d\mathbf{k}. \tag{4.36b}$$

To complete the list we quote the expression for the relativity ("boost") generators, which take the form

$$\mathfrak{K} = \sum_{\lambda=+,-} \int a_\lambda^\dagger(\mathbf{k}) \mathbf{K}_\lambda a_\lambda(\mathbf{k})\, d\mathbf{k}, \tag{4.37}$$

where

$$\mathbf{K}_\lambda = -\frac{i}{2}\left\{ \frac{\partial}{\partial \mathbf{k}} E_\lambda(k) + E_\lambda(k) \frac{\partial}{\partial \mathbf{k}} \right\}. \tag{4.38}$$

It is simple to verify that the proper commutation relations are satisfied by these generators. As usual, the restriction on the functional form of $E_\lambda(k)$ follows from the requirement that

$$\mathfrak{P} = i[\mathfrak{K}; H]. \tag{4.39}$$

To satisfy this condition we require that

$$\begin{aligned}\mathbf{k} &= \left[E_\lambda(k) \frac{\partial}{\partial \mathbf{k}}, E_\lambda(k) \right] \\ &= \frac{1}{2} \frac{\partial}{\partial \mathbf{k}} E_\lambda^2(k). \end{aligned} \tag{4.40}$$

The solutions $E_\lambda^2(k) = k^2 + \mu_\lambda^2$ are consistent with either the positive or indefinite energy case discussed above.

Weak Correspondence Principle

According to the weak correspondence principle, the expression

$$H(f, g) \equiv \langle f, g |\, H \,| f, g \rangle \tag{4.41}$$

coincides with the classical Hamiltonian where f and g play the role of the classical momentum and field, respectively.[14] If we make use of the relations

$$a_1(\mathbf{k}) \,| f, g \rangle = 2^{-\frac{1}{2}}[\alpha^{\frac{1}{2}}(k)\tilde{f}(\mathbf{k}) - i\alpha^{-\frac{1}{2}}(k)\tilde{g}(\mathbf{k})] \,| f, g \rangle, \tag{4.42a}$$

$$a_2(\mathbf{k}) \,| f, g \rangle = -i(2)^{-\frac{1}{2}}\gamma^{\frac{1}{2}}(k)\tilde{g}(\mathbf{k}) \,| f, g \rangle, \tag{4.42b}$$

it follows from (4.4) and (3.9) that

$$\begin{aligned} H_0(f, g) &= \langle f, g |\, H_0 \,| f, g \rangle \\ &= \tfrac{1}{2}\int \{ |\tilde{f}(\mathbf{k})|^2 + (\beta^2 + r\beta - r/\alpha)\, |\tilde{g}(\mathbf{k})|^2 \}\, d\mathbf{k}. \end{aligned} \tag{4.43}$$

An alternate expression for the factor in this equation

[13] For the structure of these representations see, e.g., A. S. Wightman, "L'invariance dans la mechanique quantique relativiste," in *Relations de dispersion et particules elémentaries* (Hermann & Cie., Paris, 1960); L. Streit, Helv. Phys. Acta **39**, 65 (1966).

[14] J. R. Klauder, J. Math. Phys. **8**, 2392 (1967).

is provided by (4.28), i.e.,

$$\Omega^2(k) = E_+^2(k)\rho_+(k) + E_-^2(k)\rho_-(k) = \beta^2 + r\beta - r/\alpha. \tag{4.44}$$

For a relativistic theory we should have

$$\Omega^2(k) = \omega^2(k) = k^2 + m_0^2, \tag{4.45}$$

where m_0^2 is a constant. In the case of an irreducible representation ($\alpha\beta = 1$, $r \neq \beta$), we automatically find $\rho_+(k) = 1$ and so need only fulfill

$$\omega(k) = \beta(k) = E_+(k). \tag{4.46}$$

In a sense, the weak correspondence principle can be said to imply covariance in this case. In the case of a reducible representation, on the other hand, the weak correspondence principle by itself does not imply covariance since it is but one condition on the three functions E_+, E_-, and ρ_+. If we were to require in addition that

$$E_\pm^2 = k^2 + \mu_\pm^2, \tag{4.47}$$

then

$$\omega^2 = k^2 + \mu_+^2\rho_+(k) + \mu_-^2\rho_-(k). \tag{4.48}$$

This leads to the independence of $\rho_\pm$ on k, and shows that

$$m_0^2 = \mu_+^2\rho_+ + \mu_-^2\rho_-, \tag{4.49}$$

which is the customary definition of the bare mass.[15] This familiar example should help make the weak correspondence principle plausible. In any case, even when the theory is not relativistically covariant, we see from (4.44) that the "classical dispersion relation" $\Omega^2(k)$ is always given as a weighted average of the "quantum dispersion relations" $E_\lambda^2(k)$.

Locality of the Hamiltonian

In this section we determine those Hamiltonians H_0 which act locally on the field $\varphi(\mathbf{x}, t)$ in the sense that

$$[\varphi^{(r)}(\mathbf{x}, t), \varphi^{(s)}(\mathbf{y}, t)] = 0, \quad \mathbf{x} \neq \mathbf{y}, \tag{4.50}$$

for all $r, s = 0, 1, 2, \cdots$, where

$$\varphi^{(r)}(\mathbf{x}, t) \equiv \frac{\partial^r \varphi(\mathbf{x}, t)}{\partial t^r} = i^r[H_0, [H_0, \cdots, [H_0, \varphi(\mathbf{x}, t)]\cdots]]. \tag{4.51}$$

From the normal mode decomposition

$$\varphi(\mathbf{x}, t) = \frac{1}{(2)^{\frac{1}{2}}(2\pi)^{\frac{3}{2}}} \int e^{i\mathbf{k}\cdot\mathbf{x}} \left\{ e^{-iE_+t}\left(\frac{\rho_+}{E_+}\right)^{\frac{1}{2}} a_+ - e^{-iE_-t}\left(\frac{\rho_-}{E_-}\right)^{\frac{1}{2}} a_- \right\} d\mathbf{k} + \text{h.c.}, \tag{4.52}$$

an expression for $\varphi^{(r)}(\mathbf{x}, t)$ can easily be obtained. From such an expression it follows in a straightforward manner that

$$[\varphi^{(r)}(\mathbf{x}, t), \varphi^{(s)}(\mathbf{y}, t)] = \frac{i^{r+s}[(-1)^r - (-1)^s]}{2(2\pi)^3} \times \int e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}[E_+^{r+s-1}\rho_+ + E_-^{r+s-1}\rho_-]\, d\mathbf{k}. \tag{4.53}$$

The desired commutativity for $\mathbf{x} \neq \mathbf{y}$ is assured if and only if[16]

$$E_+^{2n}\rho_+ + E_-^{2n}\rho_- = P_n, \tag{4.54}$$

for $n = 1, 2, \cdots$, where P_n is a polynomial in k^2. We may invert these relations so as to find an expression for $E_\pm^2$ in terms of the first few P_n. To find this expression we note that $E_\pm$ must be solutions of a biquadratic $E_\pm^4 + BE_\pm^2 + C = 0$. Averaging this relation, as well as one obtained by premultiplication with $E_\pm^2$, with $\rho_\pm$ and using (4.54) permit us to find B and C as functions of P_1, P_2, and P_3. In particular, we learn that

$$(P_2 - P_1^2)E_\pm^4 + (P_1P_2 - P_3)E_\pm^2 + P_1P_3 - P_2^2 = 0. \tag{4.55}$$

The solution of (4.55) has the form

$$E_\pm^2 = R_1 \pm (R_2)^{\frac{1}{2}}, \tag{4.56}$$

where R_1 and R_2 are rational functions of k^2. In addition, we have

$$\rho_+ = \tfrac{1}{2}[1 + (P_1 - R_1)/(R_2)^{\frac{1}{2}}]. \tag{4.57}$$

Using these relations to extend Eq. (4.54) into the complex k^2 plane, we see that R_1 and R_2 must in fact be polynomials since the infinities that would arise could not cancel for all values of n. With this understanding, Eqs. (4.56) and (4.57) represent the most general solution to (4.54) when $E_+^2 \neq E_-^2$ and $\rho_+ \neq 0, 1$.

Further restrictions on the R_j follow from the self-adjointness of H_0 and the existence of CCR. Since $E_\pm^2 > 0$, we must have

$$R_1^2(k^2) > R_2(k^2) > 0 \tag{4.58}$$

for almost all k^2. The remaining physical requirements are fulfilled, provided that

$$E_\pm\rho_\pm = \tfrac{1}{2}[R_1 \pm (R_2)^{\frac{1}{2}}]^{\frac{1}{2}}[1 \pm (P_1 - R_1)/(R_2)^{\frac{1}{2}}] > 0. \tag{4.59}$$

In the degenerate cases, where $\rho_+ = 0, 1$ or $E_+ = \pm E_-$, all except $E_+ = -E_-$ amount to $\alpha\beta = 1$. To

[15] See, e.g., S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper and Row Publishers, Inc., New York, 1962), p. 659.

[16] L. Schwartz, *Theorie des distributions* (Hermann & Cie., Paris, 1950), Vol. 1, Theorem XXXV, p. 99.

achieve locality (in our sense) requires that (the nondegenerate) E^2 be a polynomial in k^2. If $E_+ = -E_-$, there is no restriction on ρ_+ (other than $\rho_+ > 1$) and our type of locality is ensured if E_+^2 $(= E_-^2)$ is a polynomial in k^2.

Hamiltonian Density

It is intuitively plausible in the local cases we are considering that the Hamiltonian H_0 may be written as the integral of a density function $H_0(\mathbf{x})$ which is local in the sense that

$$[H_0(\mathbf{x}), H_0(\mathbf{y})] = 0 \tag{4.60}$$

and relatively local in the sense that

$$[H_0(\mathbf{x}), \varphi(\mathbf{y})] = [H_0(\mathbf{x}), \pi(\mathbf{y})] = 0 \tag{4.61}$$

for $\mathbf{x} \neq \mathbf{y}$. This notion can be established by the following argument. The Jacobi identity states that

$$[[H_0(\mathbf{x}), H_0(\mathbf{y})], \varphi^{(m)}(\mathbf{z})] + [[\varphi^{(m)}(\mathbf{z}), H_0(\mathbf{x})], H_0(\mathbf{y})] + [[H_0(\mathbf{y}), \varphi^{(m)}(\mathbf{z})], H_0(\mathbf{x})] = 0, \tag{4.62}$$

where $\varphi^{(m)}(\mathbf{z}) = \partial^m \varphi(\mathbf{z})/\partial t^m$. Whenever $\mathbf{x} \neq \mathbf{y}$, the local density concept implies the vanishing of the last two double commutators, for then $\mathbf{x}$ and $\mathbf{y}$ can not *both* equal $\mathbf{z}$ as is required for nonvanishing values. Accordingly, the first double commutator vanishes for all m and $\mathbf{z}$, which implies that for $\mathbf{x} \neq \mathbf{y}$ the commutator $[H_0(\mathbf{x}), H_0(\mathbf{y})]$ is a c number which must vanish for strictly quadratic Hamiltonian densities.

In the case of an irreducible CCR representation the desired local density $H_0(\mathbf{x})$ is easily established. Without loss of generality we assume $\rho_+ = 1$ and thus $(a_+ = a, E_+ = E)$

$$H_0 = \int a^\dagger(\mathbf{k}) E(k) a(\mathbf{k})\, d\mathbf{k}. \tag{4.63}$$

Employing the relation

$$\varphi(\mathbf{x}, t) = \frac{1}{(2)^{\frac{1}{2}}} \frac{1}{(2\pi)^{\frac{3}{2}}} \int e^{i(\mathbf{k}\cdot\mathbf{x} - Et)} a(\mathbf{k}) \frac{d\mathbf{k}}{[E(k)]^{\frac{1}{2}}} + \text{h.c.}, \tag{4.64}$$

we see that

$$H_0 = \tfrac{1}{2} \int :\pi^2(\mathbf{x}, t) + \varphi(\mathbf{x}, t) E^2(-i\nabla) \varphi(\mathbf{x}, t): d\mathbf{x}. \tag{4.65}$$

The locality condition already found—namely, that $E^2(k)$ is a polynomial in k^2—leads to a manifestly local Hamiltonian density $H_0(\mathbf{x})$ since the separate terms $:\pi^2:$ and $:\varphi E^2 \varphi:$ are individually and mutually local (in a formal sense).

The analogous problem in the case of a reducible CCR representation is much more complicated. While it may be expected that the Hamiltonian could be expressed as a quadratic form in $\varphi(\mathbf{x})$ and $\pi(\mathbf{x})$, this expectation is incorrect, as we shall see. What is true, however, is that the Hamiltonian may be expressed as a quadratic form in the *two* basic canonical pairs $(\lambda = +, -)$

$$\varphi_\lambda(\mathbf{x}) = \frac{1}{(2)^{\frac{1}{2}}(2\pi)^{\frac{3}{2}}} \int e^{i\mathbf{k}\cdot\mathbf{x}} a_\lambda(\mathbf{k}) \frac{d\mathbf{k}}{[E_\lambda(k)]^{\frac{1}{2}}} + \text{h.c.}, \tag{4.66a}$$

$$\pi_\lambda(\mathbf{x}) = \frac{-i}{(2)^{\frac{1}{2}}(2\pi)^{\frac{3}{2}}} \int e^{i\mathbf{k}\cdot\mathbf{x}} a_\lambda(\mathbf{k}) [E_\lambda(k)]^{\frac{1}{2}}\, d\mathbf{k} + \text{h.c.} \tag{4.66b}$$

In particular, we find directly from (4.16) that

$$H_0 = \tfrac{1}{2} \sum_{\lambda=+,-} \int :\pi_\lambda^2(\mathbf{x}) + \varphi_\lambda(\mathbf{x}) E_\lambda^2(-i\nabla) \varphi_\lambda(\mathbf{x}): d\mathbf{x}. \tag{4.67}$$

From this expression it is apparent that *four* fields are necessary to describe H_0: in particular, φ_λ and π_λ for $\lambda = +, -$. Moreover, the integrand in (4.67) need not be termwise local to ensure the locality of $\varphi(\mathbf{x}, t)$. For instance, the term $:\varphi_+ E_+^2 \varphi_+:$ is not necessarily local since it is not required that E_+^2 is a polynomial. An alternative expression for the Hamiltonian may be given in terms of the four fields φ, $\dot{\varphi}$, $\ddot{\varphi}$, and $\dddot{\varphi}$. However, it, too, does not exhibit manifest termwise locality. Evidently, locality of the Hamiltonian density in such cases is a property of the entire integrand.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Linear Physical Chains with Sturm–Liouville Characteristic Polynomials

F. L. COOK*
Georgia Institute of Technology and George C. Marshall Space Flight Center
AND
J. W. JAYNE†
United States Naval Academy

(Received 1 August 1968)

This paper deals with the existence and construction of linear physical chains whose characteristic (secular) polynomials are essentially one of four classical types: Hermite, generalized Laguerre, generalized Bessel, or Jacobi. Each of the results is useful for determining the natural frequencies (normal frequencies or eigenvalues) of the systems involved. A chain of coupled harmonic oscillators or the corresponding electrical analog can be regarded as a prototype of the systems under consideration. Chains of both arbitrary finite order and infinite order are considered. Let N be a prespecified positive integer. Consider a finite sequence $\{S_n\}_{n=1}^{N}$ of linear dissipationless spring–mass chains in which S_n consists of masses $m_0, m_1, \cdots, m_{n-1}$ and springs with spring constants $k_0, k_1, \cdots, k_n$, and in which S_{n+1} is obtained from S_n by attaching mass m_n and spring with spring constant k_{n+1}. S_n is connected to a wall by the spring having spring constant k_n, but the chain may be free at the other end. In this case S_1 is to consist only of mass m_0 and spring with spring constant k_1. Three major results relating to such a sequence are obtained. First, given a positive integer N, a procedure is developed whereby an existing Nth-order spring–mass system can readily be tested to determine whether the characteristic polynomials $\phi_1, \phi_2, \cdots, \phi_N$ associated with chains $S_1, S_2, \cdots, S_N$ are all classical polynomials of a single type; and if so, which type. The testing procedure can also be extended to the infinite-order case. Secondly, by means of large classes of examples, it is demonstrated that physical systems of any preassigned order N can actually be constructed so that for $1 \leq n \leq N$ the characteristic polynomials of S_n are all a specified one of the four classical types. Finally, it is shown that of the four possible kinds, only Jacobi- and Laguerre-type infinite-order systems can be generated; and the latter type can occur only if relatively stringent conditions on the physical parameters are satisfied.

INTRODUCTION

In the analysis of certain classes of coupled linear systems, of which a chain of coupled linear harmonic oscillators or its corresponding electrical analog may be regarded as a prototype, an important problem consists of determining the natural frequencies (normal frequencies or eigenvalues) of the systems. These frequencies are found by calculating the zeros of the characteristic (secular) polynomial for the system, where the characteristic polynomial is that polynomial which, when equated to zero, yields the characteristic (secular) equation of the system.

Three questions related to determination of the zeros of characteristic polynomials for the physical systems under consideration are answered in this paper. Their formulation is made with reference to the spring–mass configuration depicted in Fig. 1. The system indicated is to be dissipationless, and the springs are linear and massless. The term k_0 may be zero; all other k_n and all m_n are to be positive.

Starting with a mass m_0 and two springs having spring constants k_0 and k_1, one can, by successively adding a mass m_j and spring with spring constant

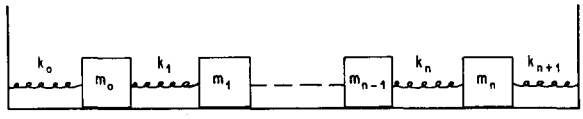


FIG. 1. Spring–mass configuration.

k_{j+1}, construct a finite sequence $\{S_n\}_{n=1}^{N}$ of spring–mass systems. The questions to be answered are as follows.

(i) Given a positive integer N, can an existing spring–mass chain containing N masses be readily tested to determine whether the characteristic polynomials $\phi_1, \phi_2, \cdots, \phi_N$ associated with subsystems $S_1, S_2, \cdots, S_N$ are all classical polynomials of a single type; and if so, which type?

(ii) Given a positive integer N, is it possible to choose positive spring constants (except possibly for k_0) and positive masses so that the characteristic polynomials of $\{S_n\}_{n=1}^{N}$ are all of a single specified classical type?

(iii) In the limiting infinite-order case, what answers, if any, can be obtained to questions analogous to those posed in (i) and (ii)?

Here, as in all that follows, a classical polynomial is understood to be a Hermite, generalized Laguerre, generalized Bessel, or Jacobi polynomial, with linear changes of argument being permitted; however, the

* Present address: Mathematics Department, University of Alabama in Huntsville, Huntsville, Alabama.
† Present address: Mathematics Department, University of Tennessee at Chattanooga, Chattanooga, Tennessee.

last three types are to be understood in a slightly extended sense from the "usual" definitions. These extensions are specified in following pages.

In Sec. 3, question (i) is affirmatively answered and the applicable testing procedure is presented. The affirmative answer to (ii) is given in Secs. 4 and 5 by means of constructed classes of examples; and the answers to (iii) are provided in Sec. 6. The development of these answers depends basically on some recent results concerning certain recursively generated polynomials.[1,2] Consequently, a summary of these results (the central one being Theorem 1.3 below) is presented in Sec. 1; the recursive relations for characteristic polynomials of the systems under consideration are then derived in Sec. 2.

1. PRELIMINARY THEOREMS AND DEFINITIONS

Let $\{\phi_n(x)\}_{n=0}^{\infty}$ be a sequence of polynomials generated by the three-term recursive relation

$$\begin{aligned} \phi_0(x) &= 1, \\ \phi_1(x) &= A_0x + B_0, \\ \phi_{n+1}(x) &= (A_nx + B_n)\phi_n(x) - C_n\phi_{n-1}(x), \quad n \geq 1, \end{aligned} \tag{1.1}$$

in which $A_0 \neq 0$, $A_nC_n \neq 0$ for $n \geq 1$, and both x and the coefficients A_i, B_i, C_i may be complex. Then ϕ_n is of degree n for each integer $n \geq 0$. It is well known[3,4] that the four kinds of polynomials under consideration are Sturm–Liouville polynomials associated with a linear second-order ordinary differential equation. Consequently, in this paper attention is confined to sequences generated as in (1.1), whose terms satisfy a differential equation of this type.

Let N be any integer greater than or equal to 3 and consider the related finite sequence $\{\phi_n(x)\}_{n=0}^{N}$ that is obtained from $\{\phi_n(x)\}_{n=0}^{\infty}$ by restricting index n to $0 \leq n \leq N$. The results of this section are applicable to both types of sequences, but they are stated only for the finite case. The corresponding statement for the infinite case can be obtained from that for the finite case merely by letting N tend to infinity in all places where it appears. Proofs of these results can be found in Refs. 1 (Chap. 4) and 2; the proofs in the finite case differ from those in the infinite case only by appropriate changes in the range of the indices.

Theorem 1.1: Suppose that for $0 \leq n \leq N$, $\phi_n(x)$ is a solution of

$$a_0(x)y'' + a_1(x)y' + [a_2(x) + \mu_n]y = 0, \tag{1.2}$$

where the prime denotes differentiation with respect to the x coordinate and where μ_n is a parameter depending on n but not on x. Then

(i) $a_2(x) + \mu_n \equiv \lambda_n = n(n-1)\lambda_2/2 - n(n-2)\lambda_1$, $0 \leq n \leq N$,

(ii) $a_1(x) \equiv \epsilon x + \delta \equiv -\lambda_1(x + b_0)$,

and

$$\begin{aligned} \text{(iii)}\ a_0(x) &\equiv \gamma x^2 + \beta x + \alpha \\ &\equiv (\lambda_1 - \lambda_2/2)x^2 \\ &\quad + [\lambda_1(b_1 + 3b_0) - \lambda_2(b_1 + b_0)]x/2 \\ &\quad + [\lambda_1(b_0b_1 + b_0^2) - \lambda_2(b_0b_1 - c_1)]/2, \end{aligned}$$

where $b_n = B_n/A_n$ for $0 \leq n \leq N-1$ and $c_n = C_n/A_nA_{n-1}$ for $1 \leq n \leq N-1$.

In the sequel, whenever reference is made to the differential equation (1.2), it is understood that the coefficient functions have the values prescribed by Theorem 1.1.

Definition 1.1: Define Δ, $g_1(n)$, and $g_2(n)$ for $1 \leq n \leq N-2$ by

$$\begin{aligned} \text{(i)}\ \Delta &= (2b_2 - b_1 - b_0) \\ &\quad \times [(b_1 - b_0)^2 + 4(c_1 + c_2)] + 9c_2(b_0 - b_2), \\ \text{(ii)}\ g_1(n) &= [(n+1)\lambda_2 - (2n+1)\lambda_1]b_{n+1} \\ &\quad - [(n-1)\lambda_2 - (2n-3)\lambda_1]b_n \\ &\quad - (b_0 + b_1)\lambda_2 + (b_1 + 3b_0)\lambda_1, \\ \text{(iii)}\ g_2(n) &= [4n\lambda_1 - (2n+1)\lambda_2]c_{n+1} \\ &\quad + [(2n-3)\lambda_2 - (4n-8)\lambda_1]c_n \\ &\quad + [(2n-1)\lambda_1 - n\lambda_2]b_n^2 \\ &\quad + [(n+1)\lambda_2 - (2n+1)\lambda_1]b_nb_{n+1} \\ &\quad - (b_0b_1 - c_1)\lambda_2 + (b_0b_1 + b_0^2)\lambda_1. \end{aligned}$$

Theorem 1.2: The polynomial $\phi_n(x)$ is a solution of (1.2) for $0 \leq n \leq N$ if and only if $g_1(n) = g_2(n) = 0$ for $1 \leq n \leq N-2$.

Differential equation (1.2) is guaranteed to be nontrivial (the coefficient functions are not all zero) provided $\Delta = 0$; and in this case the choices $\lambda_1 = 1$ and $\lambda_2 = [(b_1 - b_0)^2 + 4(c_1 + c_2)]/3c_2$ can be made without loss in generality. These values of λ_1 and λ_2 and the condition $\Delta = 0$ are assumed in all that

[1] F. L. Cook, Ph.D. dissertation, Georgia Institute of Technology, 1967.
[2] D. V. Ho, J. W. Jayne, and M. B. Sledd, Duke Math. J. 33, 131 (1966).
[3] H. L. Krall and O. Frink, Trans. Am. Math. Soc. 65, 100 (1949).
[4] G. Szegö, *Orthogonal Polynomials* (American Mathematical Society, Providence, R.I., 1959), Colloquiums Publication, Vol. XXIII.

follows. Also, the restrictions $\lambda_i \neq \lambda_j$ $(i \neq j;\ i, j = 0, 1, 2, \cdots, N)$ are of great importance in ensuing work. With $\lambda_0 = 0$ and $\lambda_1 = 1$ they are equivalent to $\lambda_2 \neq 2(i+j-2)/(i+j-1)$, $i \neq j;\ i+j \geq 2,\ i, j = 0, 1, 2, \cdots, N$. Under such restrictions the system of difference equations $g_1(n) = g_2(n) = 0$, $1 \leq n \leq N-2$, has no singular points; and the (unique) solution (for given b_0, b_1, c_1, and λ_2) is known (Ref. 1, Chap. 4). It is given by

$$b_n = \frac{[(b_0 + b_1)(\lambda_2 - 2) + (b_1 - b_0)][(n-1)(\lambda_2 - 2) + 2]n - 2b_0(\lambda_2 - 2) + 2b_0}{2[n(\lambda_2 - 2) + 1][(n-1)(\lambda_2 - 2) + 1]}, \tag{1.3}$$

$$c_n = \frac{n[(n-2)(\lambda_2 - 2) + 2]}{[(2n-1)(\lambda_2 - 2) + 2][(2n-3)(\lambda_2 - 2) + 2]} \times \left\{\lambda_2 c_1 + (b_1 - b_0)^2(\lambda_2 - 1)^2(n-1)\frac{(n-1)(\lambda_2 - 2) + 2}{4[(n-1)(\lambda_2 - 2) + 1]^2}\right\}, \quad 2 \leq n \leq N-1. \tag{1.4}$$

Remark 1.1: For the limiting infinite-order case, it is known (Ref. 5, Chap. 3) that whenever $\phi_n(x)$ satisfies the nontrivial differential equation (1.2) for $n \geq 0$, it is impossible for λ_i to equal λ_j with $i \neq j$. Hence, no singular points of the system $g_1(n) = g_2(n) = 0$, $n \geq 1$, can occur; and the solution is given by (1.3) and (1.4) for $n \geq 2$. On the other hand, the situation $\lambda_i = \lambda_j$ for unequal integers i and j in $[0, N]$ can occur if $\phi_n(x)$ satisfies (1.2) only for $0 \leq n \leq N$ (Ref. 1, Chap. 3). Even in this case the solution to the finite system $g_1(n) = g_2(n) = 0$, $1 \leq n \leq N-2$, (provided it exists) has been determined. Equation (1.4) and some results of Ref. 5 can be used to provide a derivation of this solution.

Theorem 1.2 and the results following can be summarized as a single theorem.

Theorem 1.3: For $0 \leq n \leq N$, $\phi_n(x)$ is a solution of the nontrivial differential equation (1.2) in which $\lambda_i \neq \lambda_j$, $i \neq j;\ i, j = 0, 1, 2, \cdots, N$ if and only if

(i) $\Delta = 0$,

(ii) $[(b_0 - b_1)^2 + 4(c_1 + c_2)]/3c_2$ is different from $2(m-2)/(m-1)$ for $2 \leq m \leq 2N-1$,

(iii) b_n and c_n are given by Eqs. (1.3) and (1.4) in which $\lambda_2 = [(b_0 - b_1)^2 + 4(c_1 + c_2)]/3c_2$.

2. RECURSIVE RELATIONS FOR THE SYSTEM OF FIGURE 1

Consider again the system of coupled harmonic oscillators shown in Fig. 1. If one mass m_0 is coupled to two springs having spring constants k_0 and k_1 ($n = 0$ in Fig. 1), the equation of motion is

$$(m_0 D^2 + k_0 + k_1)x_0 = 0,$$

where $D = d/dt$ and x_0 is the displacement of m_0 from the equilibrium position. If a second mass m_1 and third spring with spring constant k_2 are added in such a way that the resulting system corresponds to $n = 1$ in Fig. 1, the equations of motion are

$$(m_0 D^2 + k_0 + k_1)x_0 - k_1 x_1 = 0,$$
$$-k_1 x_0 + (m_1 D^2 + k_1 + k_2)x_1 = 0.$$

If the system is enlarged by adding additional masses and springs in the manner indicated and if N is any integer greater than or equal to 3, the equations of motion for N masses and $N+1$ springs are

$$\begin{aligned}
(m_0 D^2 + k_0 + k_1)x_0 - k_1 x_1 &= 0,\\
-k_1 x_0 + (m_1 D^2 + k_1 + k_2)x_1 - k_2 x_2 &= 0,\\
&\vdots\\
-k_n x_{n-1} + (m_n D^2 + k_n + k_{n+1})x_n - k_{n+1}x_{n+1} &= 0,\\
&\vdots\\
-k_{N-1}x_{N-2} + (m_{N-1}D^2 + k_{N-1} + k_N)x_{N-1} &= 0.
\end{aligned} \tag{2.1}$$

To obtain the finite sequence $\{\phi_n\}_{n=1}^N$ of characteristic polynomials associated with this finite sequence $\{S_n\}_{n=1}^N$ of successively larger spring–mass configurations, assume solutions of the form $x_j = T_j e^{i\omega t}$, substitute into the appropriate-size system of differential equations, and then expand the resultant determinant of the coefficient matrix of the system. If each of the nth-order determinants $(1 \leq n \leq N)$ is expanded about its last row, the results are

$$\begin{aligned}
\phi_1 &= -m_0\omega^2 + k_0 + k_1,\\
\phi_2 &= (-m_1\omega^2 + k_1 + k_2)\phi_1 - k_1^2,\\
\phi_3 &= (-m_2\omega^2 + k_2 + k_3)\phi_2 - k_2^2\phi_1,\\
&\vdots\\
\phi_n &= (-m_{n-1}\omega^2 + k_{n-1} + k_n)\phi_{n-1} - k_{n-1}^2\phi_{n-2},\\
&\vdots\\
\phi_N &= (-m_{N-1}\omega^2 + k_{N-1} + k_N)\phi_{N-1} - k_{N-1}^2\phi_{N-2}.
\end{aligned} \tag{2.2}$$

[5] J. W. Jayne, Ph.D. dissertation, Georgia Institute of Technology, 1965.

Thus, if ϕ_0 is defined to be 1 and if the characteristic polynomials for the systems of orders $n-1$, n, and $n+1$ are viewed as polynomials in ω^2, they are related by a three-term recurrence relation of the form (1.1), in which

$$b_n = -(k_n + k_{n+1})/m_n, \quad 0 \leq n \leq N-1, \quad (2.3)$$

and

$$c_n = k_n^2/m_n m_{n-1}, \quad 1 \leq n \leq N-1. \quad (2.4)$$

Consequently, each b_n is negative and each c_n is positive for this finite sequence of systems. The value of λ_2 to be used is $[(b_1 - b_0)^2 + 4(c_1 + c_2)]/3c_2$ (recall the discussion immediately following Theorem 1.2), where b_0, b_1, c_1, and c_2 are as specified in Eqs. (2.3) and (2.4).

Remark 2.1: Our attention has been called to the following interesting physical interpretation for the characteristic polynomials of this sequence of systems; a more detailed discussion can be found in Ref. 6. Suppose $k_0 > 0$ (so that the system of Fig. 1 is fastened at both ends) and let u_n denote the displacement amplitude of mass m_n. Set $u_0 = 1$. Then u_n, thought of as a function of parameter ω^2, is related to ϕ_n by $\phi_0(\omega^2) = u_0(\omega^2)$ and $\phi_n(\omega^2) = k_1 k_2 \cdots k_n u_n(\omega^2)$ if $n \geq 1$. For a given system S_N of order $N \geq 3$, $\phi_0(\omega^2) = u_0(\omega^2)$, $\phi_n(\omega^2) = k_1 k_2 \cdots k_n u_n(\omega^2)$ if $1 \leq n \leq N-1$, and $\phi_N(\omega^2) = k_1 k_2 \cdots k_N u_N(\omega^2)$, where u_N is the displacement amplitude of the last mass m_N in system S_{N+1} of order $N+1$. Thus, the zeros of $u_N(\omega^2)$ are precisely the squared natural frequencies of system S_N.

For the electrical analog of the system depicted in Fig. 1, the differential equations and characteristic polynomials are readily obtained from (2.1) and (2.2) by replacing m_i, k_i, and x_i by inductance L_i, the reciprocal of capacitance, D_i, and charge Q_i, respectively—the analogy being drawn only if $k_0 > 0$. In this case conditions (2.3) and (2.4) become

$$b_n = -(D_n + D_{n+1})/D_n D_{n+1} L_n, \quad 0 \leq n \leq N-1, \quad (2.5)$$

and

$$c_n = (D_n^2 L_n L_{n-1})^{-1}, \quad 1 \leq n \leq N-1. \quad (2.6)$$

Once again, each b_n is negative, each c_n is positive, and λ_2 is computed from $[(b_1 - b_0)^2 + 4(c_1 + c_2)]/3c_2$.

[6] H. B. Rosenstock and R. E. McGill, J. Math. Phys. 3, 200 (1962).

3. CHARACTERIZATION OF HERMITE, LAGUERRE, BESSEL, AND JACOBI POLYNOMIAL SEQUENCES

The following four pairs of theorems provide necessary and sufficient conditions that a sequence $\{\phi_n(x)\}_{n=0}^{\infty}$ generated as in (1.1) or its related finite sequence $\{\phi_n(x)\}_{n=0}^{N}$ ($N \geq 3$) be—apart from a determinable linear change of variable and computable multiplicative factors independent of x—a sequence (finite sequence) of one of the four types of classical polynomials. The conditions are formulated in terms of only the coefficients b_n and c_n, which are defined in Theorem 1.1. Consequently, question (i) and the portion of question (iii) related to question (i) can be answered by use of these theorems in which b_n and c_n are identified as in (2.3) and (2.4).

For efficiency in application, the theorems are stated separately rather than lumped into "if and only if" theorems. Moreover, proofs are provided for only two of the four pairs (the Hermite and Jacobi cases) because techniques used are much the same in all four cases. Proofs for the remaining two pairs can be found in Ref. 1, Chap. 3. Finally, as in Sec. 1, results are stated only for the finite case with arbitrary $N \geq 3$; extensions to the infinite case can be obtained in the natural manner.

In all that follows, N is a fixed but arbitrary integer not less than 3, and D_n denotes a nonzero term independent of x.

Definition 3.1: Let n be a nonnegative integer. The Hermite polynomial of degree n, denoted by H_n, is defined by

$$H_n(t) = \sum_{k=0}^{[n/2]} \frac{(-1)^k n!\,(2t)^{n-2k}}{k!\,(n-2k)!},$$

where [ ] denotes the greatest integer function.

Theorem 3.1: If (A) $\lambda_2 = 2$, (B) $b_1 = b_0$, and (C) b_n and c_n are given by (1.3) and (1.4) for $2 \leq n \leq N-1$, then $\phi_n(x) = D_n H_n((x + b_0)(2c_1)^{-\frac{1}{2}})$ for $0 \leq n \leq N$, where the principal square root is taken.

Proof: If conditions A–C hold, Theorem 1.3 implies that $\phi_n(x)$ satisfies a differential equation of the form (1.2) in which $\lambda_1 = 1$, $\lambda_2 = 2$, and $b_1 = b_0$. Consequently, $\phi_n(x)$ is a solution of

$$c_1 y'' - (x + b_0)y' + ny = 0 \quad (3.1)$$

(where the prime denotes d/dx) for $0 \leq n \leq N$. Under the change of variable $x = (2c_1)^{\frac{1}{2}}t - b_0$, where the principal square root is taken, (3.1) transforms to the Hermite differential equation

$$y'' - 2ty' + 2ny = 0, \quad (3.2)$$

where the prime denotes d/dt. The only polynomial solutions of (3.2) are (to within multiplicative constants) the Hermite polynomials. Hence,

$$\phi_n(x) = D_n H_n((x + b_0)(2c_1)^{-\frac{1}{2}}) \quad \text{for} \quad 0 \leq n \leq N.$$

Theorem 3.2: If there exist a nonzero constant μ and a constant ν such that $\phi_n(x) = D_n H_n(\mu x + \nu)$ for $0 \leq n \leq N$, then b_n and c_n satisfy conditions A–C of Theorem 3.1.

Proof: Whenever such constants exist, it follows from (3.2) and the chain rule for differentiation that $\phi_n(x)$ is a solution of

$$(2\mu^2)^{-1}y'' + (-x - \nu/\mu)y' + ny = 0 \qquad (3.3)$$

(where the prime denotes d/dx) for $0 \leq n \leq N$. Equation (3.3) is a nontrivial differential equation of the form (1.2) in which $\lambda_1 = 1$ and $\lambda_2 = 2$. Hence, by Theorem 1.3, condition C is satisfied; and from part (iii) of Theorem 1.1, $0 = \beta = (b_0 - b_1)/2$.

Definition 3.2: Let n be a nonnegative integer and a any complex number. The extended generalized Laguerre polynomial of degree n, denoted by L_n^a, is defined by

$$L_n^a(t) = \sum_{k=0}^{n} \binom{a+n}{n-k}(-1)^k t^k/k!,$$

where

$$\binom{a+n}{n-k} = \prod_{j=1}^{n-k} (a + k + j)/(n - k)!$$

if $0 \leq k \leq n - 1$ and $\binom{a+n}{0} = 1$.

The definition of L_n^a given here agrees with that of the classical generalized Laguerre polynomial of degree n whenever $a > -1$.

Theorem 3.3: If (A) $\lambda_2 = 2$, (B) $b_1 \neq b_0$, and (C) b_n and c_n are given by (1.3) and (1.4) for $2 \leq n \leq N - 1$, then for $0 \leq n \leq N$, $\phi_n(x) = D_n L_n^a(\mu x + \nu)$, where $a = 4c_1(b_0 - b_1)^{-2} - 1$, $\mu = 2/(b_0 - b_1)$, and $\nu = 2(b_0 + 2c_1/(b_0 - b_1))/(b_0 - b_1)$.

Theorem 3.4: If there exist a nonzero constant μ and constants ν and a such that $\phi_n(x) = D_n L_n^a(\mu x + \nu)$ for $0 \leq n \leq N$, then b_n and c_n satisfy conditions A–C of Theorem 3.3.

Definition 3.3: Let n be a positive integer, b a nonzero complex number, and a a complex number not an integer in $[-2(n - 1), -(n - 1)]$. The extended generalized Bessel polynomial of degree n, denoted by $B_n^{(a,b)}$, is defined by

$$B_n^{(a,b)}(t) = \sum_{k=0}^{n} \binom{n}{k}(n + k + a - 2)^{(k)} \left(\frac{t}{b}\right)^k,$$

where $\binom{n}{k}$ is a binomial coefficient,

$$(n + k + a - 2)^{(k)} = \prod_{j=1}^{k} (n + k + a - j - 1)$$

if $1 \leq k \leq n$, and $(n + a - 2)^{(0)} = 1$. For nonzero complex b, $B_0^{(a,b)}(t) \equiv 1$.

The definition above agrees with that of the generalized Bessel polynomial of degree n provided a is other than a nonpositive integer.[3] The condition imposed on a for $n \geq 1$ is the minimal one to guarantee that $B_n^{(a,b)}$ is a polynomial of degree exactly n.

Theorem 3.5: If (A) $\lambda_2 \neq 2$, (B) $(\lambda_2 - 1)^2(b_0 - b_1)^2 + 4\lambda_2(\lambda_2 - 2)c_1 = 0$, (C) b_n and c_n are given by (1.3) and (1.4) for $2 \leq n \leq N - 1$, and (D) $\lambda_2 \neq 2(m - 2)/(m - 1)$ for $2 \leq m \leq 2N - 1$, then

$$\phi_n(x) = D_n B_n^{(a,2)}(\mu x + \nu) \quad \text{for} \quad 0 \leq n \leq N,$$

where

$$a = 2/(\lambda_2 - 2), \quad \mu = 2(\lambda_2 - 2)^2/(b_0 - b_1)(\lambda_2 - 1),$$

and

$$\nu = (\lambda_2 - 2)[(b_0 + b_1)\lambda_2 - (3b_0 + b_1)]/(\lambda_2 - 1)(b_0 - b_1).$$

Theorem 3.6: If there exist a nonzero constant μ and constants ν, a, and b such that

$$\phi_n(x) = D_n B_n^{(a,b)}(\mu x + \nu)$$

for $0 \leq n \leq N$, then b_n and c_n satisfy conditions A–D of Theorem 3.5.

Definition 3.4: Let n be a positive integer and let a and b be any two complex constants such that $a + b$ is not an integer in $[-2n, -(n + 1)]$. The generalized Jacobi polynomial of degree n, denoted by $P_n^{(a,b)}$, is defined by

$$P_n^{(a,b)}(t) = \frac{1}{n!}\Bigg\{\prod_{j=1}^{n}(a + j) + \sum_{k=1}^{n-1}\Bigg[\binom{n}{k}\prod_{j=1}^{k}(n + a + b + j) \times \prod_{m=1}^{n-k}(a + k + m)((t - 1)/2)^k\Bigg] + \prod_{j=1}^{n}(n + a + b + j)((t - 1)/2)^n\Bigg\},$$

where the middle summand is omitted when $n = 1$. For any two complex numbers a and b, $P_0^{(a,b)}(t) \equiv 1$.

Definition 3.4 agrees with that of the classical Jacobi polynomial of degree n provided[4] $a > -1$ and

$b > -1$. The condition imposed on $a + b$ for $n \geq 1$ is the minimal one to guarantee that $P_n^{(a,b)}$ is of degree n.

Theorem 3.7: If (A) $\lambda_2 \neq 2$, (B) $(\lambda_2 - 1)^2(b_0 - b_1)^2 + 4\lambda_2(\lambda_2 - 2)c_1 \neq 0$, (C) b_n and c_n are given by (1.3) and (1.4) for $2 \leq n \leq N - 1$, and (D) $\lambda_2 \neq 2(m - 2)/(m - 1)$ for $2 \leq m \leq 2N - 1$, then

$$\phi_n(x) = D_n P_n^{(a,b)}(1 - 2(\mu x + \nu)) \quad \text{for} \quad 0 \leq n \leq N,$$

where

$$a = -1 + 2(x_1 + b_0)/(\lambda_2 - 2)(x_1 - x_2),$$
$$b = -1 + 2(x_2 + b_0)/(\lambda_2 - 2)(x_2 - x_1),$$
$$\mu = 1/(x_2 - x_1) \quad \text{and} \quad \nu = -x_1/(x_2 - x_1).$$

Here

$$x_2 = [\lambda_2(b_0 + b_1) - (b_1 + 3b_0)]/2(2 - \lambda_2) + \{[(\lambda_2 - 1)^2(b_0 - b_1)^2 + 4\lambda_2(\lambda_2 - 2)c_1]/4(2 - \lambda_2)^2\}^{\frac{1}{2}}$$

and

$$x_1 = -x_2 + [\lambda_2(b_0 + b_1) - (b_1 + 3b_0)]/(2 - \lambda_2)$$

are the two distinct zeros of the coefficient of y'' in (1.2) (the square root used being the principal one).

Proof: If conditions A–C hold, Theorem 1.3 implies that $\phi_n(x)$ satisfies (1.2) in which $\lambda_1 = 1$, $\lambda_2 \neq 0$, and discriminant D of the coefficient of y'' is nonzero. Hence $\phi_n(x)$ is a solution of

$$(1 - \lambda_2/2)(x - x_1)(x - x_2)y'' - (x + b_0)y' + [n(n - 1)\lambda_2/2 - n(n - 2)]y = 0, \quad (3.4)$$

where the unequal quantities x_1 and x_2 are as specified in the statement of the theorem. If the change of variable $x = \frac{1}{2}[x_1 + x_2 - (x_2 - x_1)t]$ is made, (3.4) transforms to the Jacobi differential equation

$$(1 - t^2)y'' + [b - a - (a + b + 2)t]y' + n(n + a + b + 1)y = 0, \quad (3.5)$$

in which a and b are as stated in the theorem. Condition D forces $2/(\lambda_2 - 2) - 2 = a + b$ to be other than an integer in $[-2N, -2]$. With this restriction on $a + b$, a straightforward argument shows that the only polynomial solutions of (3.5) (to within multiplicative constants) are the generalized Jacobi polynomials. It follows that

$$\phi_n(x) = D_n P_n^{(a,b)}[1 - 2(x - x_1)/(x_2 - x_1)]$$

for $0 \leq n \leq N$.

Theorem 3.8: If there exist a nonzero constant μ and constants ν, a, and b such that

$$\phi_n(x) = D_n P_n^{(a,b)}[1 - 2(\mu x + \nu)] \quad \text{for} \quad 0 \leq n \leq N,$$

then b_n and c_n satisfy conditions A–D of Theorem 3.7.

Proof: From (3.5), the chain rule for differentiation, and the fact that $a + b \neq -2$, it follows that $\phi_n(x)$ is a solution of

$$\frac{(\mu x + \nu)(1 - \mu x - \nu)}{\mu^2(a + b + 2)} y'' + \left[\frac{a + 1}{\mu(a + b + 2)} - \frac{(\mu x + \nu)}{\mu}\right]y' + \frac{n(n + a + b + 1)}{a + b + 2} y = 0 \quad (3.6)$$

for $0 \leq n \leq N$. Equation (3.6) is a nontrivial differential equation of the form (1.2) in which $\lambda_1 = 1$, $\lambda_2 \neq 2$, and discriminant $D \neq 0$. By Theorem 1.3, condition C is satisfied; and since $2/(\lambda_2 - 2) - 2 = a + b$ is not an integer in $[-2N, -2]$,

$$\lambda_2 \neq 2(m - 2)/(m - 1) \quad \text{for} \quad 2 \leq m \leq 2N - 1.$$

In addition to providing constructive answers to question (i) and a portion of question (iii), Theorems 3.1–3.8 and their extensions to the infinite case indicate at what point (if any) the sequence of systems S_n first fails to meet the requirements. If all conditions are satisfied except the representations for b_n and c_n given by (1.3) and (1.4) (and condition D in the Bessel and Jacobi cases) and if j is the largest integer in $[3, N)$ such that these exceptions hold true for $2 \leq n \leq j - 1$ (and $2 \leq m \leq 2j - 1$), then systems $S_1, S_2, \cdots, S_j$ will have characteristic polynomials $\phi_n(\omega^2)$ that are all of one classical type; but the finite sequence of systems $\{S_n\}_{n=1}^{j+1}$ will not meet such requirements.

A computational advantage that occurs when a spring–mass chain is one of the four types, is the relative ease with which the natural frequencies can be determined. Since the linear change of variable and other parameters that occur in characteristic polynomial ϕ_N can readily be calculated, the problem of determining the natural frequencies of such an Nth-order system often reduces merely to looking up the N tabulated zeros of the type of polynomial involved. Even if a tabulation of the desired zeros has not been made, a numerical compilation of these zeros should not be difficult to obtain because of the detailed available knowledge about them.[4] Clearly the same comments are applicable to the j natural frequencies of any subsystem S_j, where $1 \leq j \leq N - 1$.

4. ADDITIONAL NECESSARY CONDITIONS FOR CONSTRUCTIONS

In question (i) the problem of physical realizability does not arise: the physical system is already built, so the spring constants and masses are *a priori* positive except possibly for k_0. The opposite is true in the study of question (ii). Theorems 3.1–3.8 state necessary and sufficient conditions on

$$b_n \equiv -(k_n + k_{n+1})/m_n \quad \text{and} \quad c_n \equiv k_n^2/m_n m_{n-1}$$

which are to be met in the mathematical representation of k_n and m_n; but the added physical requirements that $k_n > 0$ for $1 \leq n \leq N$, $k_0 \geq 0$, and $m_n > 0$ for $0 \leq n \leq N-1$, must also be taken into account. Such requirements imply that $b_n < 0$ for $0 \leq n \leq N-1$ and $c_n > 0$ for $1 \leq n \leq N-1$. Based on these sign constraints, the next four theorems provide additional necessary conditions for construction of an Nth-order spring–mass system of one of the desired types.

Notice first that if $\lambda_2 = 2$, Eqs. (1.3) and (1.4) reduce to

$$b_n = b_0 + (b_1 - b_0)n \tag{4.1}$$

and

$$c_n = (n^2 - n)(b_1 - b_0)^2/4 + nc_1, \tag{4.2}$$

respectively. From these relations and Theorems 3.1–3.4, the first two of the four theorems are evident. They are stated simply for completeness.

Theorem 4.1: In the Hermite case, $c_n > 0$ for $1 \leq n \leq N-1$ and $b_n < 0$ for $0 \leq n \leq N-1$ if and only if $b_0 < 0$ and $c_1 > 0$.

Theorem 4.2: In the extended generalized Laguerre case, $c_n > 0$ for $1 \leq n \leq N-1$ and $b_n < 0$ for $0 \leq n \leq N-1$ if and only if $b_0 < 0$, $b_1 < 0$, $b_1 < b_0(1 - 1/(N-1))$, and $c_1 > 0$.

Remark 4.1: At this stage it is worth noting that any Nth-order extended generalized Laguerre system which is built will be of the "usual" generalized Laguerre type (that is, $a > -1$); for by Theorems 3.3–3.4, the characteristic polynomials are $\phi_n(\omega^2) = D_n L_n^a(\mu\omega^2 + \nu)$ for $0 \leq n \leq N$, where

$$a = 4c_1/(b_0 - b_1)^2 - 1 > -1.$$

Theorem 4.3: In the extended generalized Bessel case, $c_n > 0$ for $1 \leq n \leq N-1$ and $b_n < 0$ for $0 \leq n \leq N-1$ if and only if $b_0 < 0$, $b_1 < 0$, $c_1 > 0$, $2 - 2/(2N-3) < \lambda_2 < 2$, and either

$$b_1 < b_0\left(\frac{3-\lambda_2}{\lambda_2 - 1}\right)\left\{1 - \frac{2}{[2 + (N-2)(\lambda_2 - 2)](N-1)}\right\} \tag{4.3}$$

or

$$b_0\left(\frac{3-\lambda_2}{\lambda_2 - 1}\right)\left\{1 - \frac{2}{[2 + (N-2)(\lambda_2 - 2)](N-1)}\right\} < b_1 < b_0\left(\frac{3-\lambda_2}{\lambda_2 - 1}\right)\left\{1 - \frac{2}{[2 + (N-3)(\lambda_2 - 2)](N-2)}\right\}. \tag{4.4}$$

Proof: Suppose first that $c_n > 0$ and $b_n < 0$. Then

$$(\lambda_2 - 1)^2(b_0 - b_1)^2 + 4\lambda_2(\lambda_2 - 2)c_1 = 0$$

implies $0 < \lambda_2 < 2$; and the solution for c_n displayed in (1.4) reduces to

$$c_n = \frac{c_1\lambda_2 n[(n-2)(\lambda_2 - 2) + 2]}{[(2n-1)(\lambda_2 - 2) + 2][(2n-3)(\lambda_2 - 2) + 2][(n-1)(\lambda_2 - 2) + 1]^2} \tag{4.5}$$

for $2 \leq n \leq N-1$. Write $E_n = (n-2)(\lambda_2 - 2) + 2$, $F_n = (2n-1)(\lambda_2 - 2) + 2$, and $G_n = (2n-3) \times (\lambda_2 - 2) + 2$. Since c_2, E_2, and G_2 are positive, (4.5) implies $F_2 > 0$. Thus $\lambda_2 > \frac{4}{3}$, and the inequality involving λ_2 is verified when $N = 3$. Suppose that $N \geq 4$ and E_j, F_j, and G_j are positive for some integer j satisfying $2 \leq j \leq N-2$. Then $G_{j+1} = F_j > 0$. Since $\lambda_2 < 2$, $G_n \leq E_n$ for $n \geq 1$; consequently $E_{j+1} > 0$. Since $c_{j+1} > 0$, (4.5) implies $F_{j+1} > 0$. Hence E_n, F_n, and G_n are positive for $2 \leq n \leq N-1$. It follows that $\lambda_2 > 2 - 2/(2N-3)$. To deduce (4.3) or (4.4), first set $\delta = 2 - \lambda_2$. Then $0 < \delta < 2/(2N-3)$, $0 < (n-1)\delta < 1$ for $2 \leq n \leq N-1$, and $0 < n\delta < 1$ for $2 \leq n \leq N-2$. In terms of δ, (1.3) can be written as

$$b_n = \frac{[b_1(1-\delta) - b_0(1+\delta)][2 - (n-1)\delta]n + 2b_0(1+\delta)}{2(1-n\delta)[1-(n-1)\delta]} \tag{4.6}$$

for $2 \leq n \leq N-1$; and the denominator will be positive for $2 \leq n \leq N-2$. According to whether $(N-1)\delta < 1$ or $(N-1)\delta > 1$, Eq. (4.3) or (4.4) will occur. For suppose $(N-1)\delta < 1$. Then $b_n < 0$ for $2 \leq n \leq N-1$ if and only if the numerator of (4.6) is negative for $2 \leq n \leq N-1$. This is true if and only if

$$b_1 < b_0\left(\frac{1+\delta}{1-\delta}\right)\left\{1 - \frac{2}{[2-(n-1)\delta]n}\right\},$$

which is equivalent to (4.3) since the expression in braces is a positive, strictly increasing function of n and since b_0 and b_1 are negative. If $(N-1)\delta > 1$, $b_n < 0$ for $2 \leq n \leq N-1$ if and only if the numerator of (4.6) is positive when $n = N-1$ and (4.3) holds with N replaced by $N-1$. The last statement implies inequality (4.4).

Conversely, suppose that $b_0 < 0$, $b_1 < 0$, $c_1 > 0$, $2 - 2/(2N-3) < \lambda_2 < 2$, and that either (4.3) or (4.4) holds. All steps taken in the necessity part of the proof for the derivation of (4.3) and (4.4) are reversible. So $b_n < 0$ for $0 \leq n \leq N-1$. When $2 - 2/(2N-3) < \lambda_2 < 2$, then E_n, F_n, and G_n are positive for $2 \leq n \leq N-1$. Consequently, by (4.5), $c_n > 0$ for $2 \leq n \leq N-1$.

Theorem 4.4: In the generalized Jacobi case, $c_n > 0$ for $1 \leq n \leq N-1$ and $b_n < 0$ for $0 \leq n \leq N-1$ if and only if $b_0 < 0$, $b_1 < 0$, $c_1 > 0$, $2 - 2/(2N-3) < \lambda_2$, and either (4.3) or (4.4) holds.

Proof: The proof is similar to that of Theorem 4.3 and is, therefore, omitted. A complete proof can be found in Ref. 1, Chap. 5.

Remark 4.2: It can easily be shown (Ref. 1, Chap. 5) that any physical Jacobi-type system of order N will have characteristic polynomials of the classical Jacobi type if and only if $\lambda_2 > 2$. Thus, if $2 - 2/(2N-3) < \lambda_2 < 2$ and $\lambda_2 \neq (2N-3)/(N-1)$, the characteristic polynomials all fall into the generalized Jacobi category. Such behavior is in contrast to that of physical Laguerre systems (see Remark 4.1).

5. SOME CONSTRUCTIONS OF THE FOUR TYPES OF SYSTEMS

Once b_0, b_1, c_1, and λ_2 are specified, b_n and c_n are completely determined by (1.3) and (1.4). The construction of any one of the desired systems therefore hinges on a choice of these parameters such that (1) all necessary conditions on b_n and c_n hold for the particular type system and (2) with the possible exception of $k_0 = 0$, each component of the solution pair $\{k_n, m_n\}$ to finite difference system (2.3) and (2.4) is positive. Equation (5.1) below is helpful in deducing appropriate choices.

Suppose that a proper choice of b_0, b_1, c_1, and λ_2 is made. Then $k_0 + k_1 = -m_0 b_0$ and

$$k_n^2 b_n/(k_n + k_{n+1})c_n = -m_{n-1} = (k_{n-1} + k_n)/b_{n-1},$$

for $1 \leq n \leq N-1$. If it is further assumed that k_0 is chosen as positive, the last equation can be rewritten as

$$v_{n+1} = b_{n-1}b_n(1 - 1/v_n)/c_n, \quad \text{for} \quad 1 \leq n \leq N-1, \tag{5.1}$$

where $v_{n+1} = 1 + k_{n+1}/k_n$, $0 \leq n \leq N-1$.

For the Hermite case, difference system (2.3) and (2.4) reduces to

$$k_n + k_{n+1} = -m_n b_0, \qquad 0 \leq n \leq N-1, \tag{5.2}$$

$$k_n^2 = n m_{n-1} m_n c_1, \quad 1 \leq n \leq N-1; \tag{5.3}$$

and (5.1) becomes

$$v_{n+1} = b_0^2(1 - 1/v_n)/nc_1, \quad \text{for} \quad 1 \leq n \leq N-1, \tag{5.4}$$

with $v_1 \equiv 1 + k_1/k_0$. Let $k_0 > 0$, $k_1 \geq k_0$, and $m_0 > 0$ be chosen and set $b_0 = -(k_0 + k_1)/m_0$. Then set $c_1 = kb_0^2/4(N-1)$, where k is a number in $(0, 1]$. With these choices $v_1 \geq 2$; and, by finite induction,

$$v_{n+1} = 4(N-1)(1 - 1/v_n)/k_n \geq 4/2k \geq 2,$$

for $1 \leq n \leq N-1$. Hence, $k_{n+1}/k_n \geq 1$; since $k_1 \geq k_0 > 0$, $k_n > 0$ for $0 \leq n \leq N$. Consequently, if k_n is computed from (5.4), it is positive and satisfies

$$k_n^2 = nc_1(k_{n-1} + k_n)(k_n + k_{n+1})/b_0^2, \quad \text{for} \quad 1 \leq n \leq N-1. \tag{5.5}$$

Use these quantities in (5.2) to compute m_n for $1 \leq n \leq N-1$. The m_n so calculated will all be positive; and (5.3) will be satisfied by virtue of (5.5). The indicated choices for b_0, b_1, c_1, and λ_2 thus guarantee that k_n and m_n computed by means of (5.2) and (5.3) will all be positive. By Theorem 3.1

$$\phi_n(\omega^2) = (-1)^n D_n H_n[((2N-2)/k)^{\frac{1}{2}}(\omega^2/b_0 + 1)], \quad 0 \leq n \leq N.$$

To satisfy the necessary conditions

$$(\lambda_2 - 1)^2(b_0 - b_1)^2 + 4\lambda_2(\lambda_2 - 2)c_1 = 0,$$

$\lambda_2 \neq 0$, and $\lambda_2 \neq 2$ in the Bessel case, b_0 cannot equal b_1 and b_0, b_1, c_1, and λ_2 must be related by

$$\lambda_2 = 1 \pm [4c_1/((b_0 - b_1)^2 + 4c_1)]^{\frac{1}{2}}. \tag{5.6}$$

The condition $2 - 2/(2N-3) < \lambda_2 < 2$ implies $\lambda_2 > \frac{4}{3}$; so only the positive square root is acceptable in (5.6). Set $\lambda_2 = 2 - 4/(4N+1)$. Then all necessary conditions on λ_2 are met; and, in fact, $\lambda_2 \neq 2(m-2)/(m-1)$ for $m \geq 2$. With this choice of λ_2 (5.6) implies

$$c_1 = (b_0 - b_1)^2(4N-3)^2/32(4N-1), \tag{5.7}$$

and since $(N-1)(2-\lambda_2) < 1$, the proof of Theorem 4.3 shows that b_0 and b_1 must be related by (4.3). Thus

$$b_1 < b_0 \frac{(N-2)(2N+3)(4N+5)}{(N-1)(2N+5)(4N-3)}. \quad (5.8)$$

Lemma 5.1: Let b_0, b_1, and c_1 be related by (5.7) and (5.8) and subject also to $b_0 < 0$, $b_1 < 0$. Then a choice of such quantities can be made so that $b_{n-1}b_n/c_n$, the coefficient of $(1 - 1/v_n)$ in (5.1), is not less than 4 for $1 \leq n \leq N-1$, where b_n is determined by (1.3), c_n is determined by (4.5), and $\lambda_2 = 2 - 4/(4N+1)$.

Proof: Choose $b_0 < 0$ and set

$$b_1 = 2N^3 b_0/(2N^3+1), \quad (5.9)$$

$$c_1 = (4N-3)^2 b_0^2/32(2N^3+1)^2(4N-1). \quad (5.10)$$

Then (5.7) and (5.8) hold; and a straightforward calculation shows that the proposed inequality is equivalent to

$$\begin{aligned} &8[4(N-n)+7][4(N-n)+3]\{32N^3(N-n)^2 \\ &\quad + 48N^3(N-n) + 10N^3 - 16N^2n + 8Nn^2 + 16N^2 \\ &\quad - 32Nn + 10n^2 + 24N - 15n + 5\} \\ &\quad \times \{32N^3(N-n)^2 + 112N^3(N-n) + 90N^3 \\ &\quad - 16N^2n + 8Nn^2 + 32N^2 - 48Nn + 10n^2 + 64N \\ &\quad - 35n + 30\} \geq [4(N-n)+1][4(N-n)+9] \\ &\quad \times (4N-3)^2(4N+1)^2(4Nn - 2n^2 + 5n), \\ &\qquad\qquad \text{for} \quad 1 \leq n \leq N-1. \quad (5.11) \end{aligned}$$

The minimum value for each of the two terms in braces in (5.11) occurs when $n = N-1$, and these minimum values are positive. Thus, for $1 \leq n \leq N-1$, each term in parentheses, brackets, or braces is positive. Because of this it is clear that (5.11) can be proved by verifying a modification in which all bracketed terms are deleted. Since both terms in braces are positive, the minimum value of the left side of (5.11) less the two bracketed terms occurs when $n = N-1$. The maximum value of the right side with the bracketed terms deleted also occurs when $n = N-1$. Hence, to establish the lemma it suffices to verify (5.11) less all bracketed terms when $n = N-1$. A routine computation of the last condition completes the proof.

With the aid of Lemma 5.1, examples of Bessel systems of order N can easily be provided. Choose $k_0 > 0, k_1 \geq k_0, m_0 > 0$ and set $b_0 = -(k_0 + k_1)/m_0$. Let b_1 and c_1 be given by (5.9) and (5.10), respectively. Then, from the proof of the lemma, the fact that $v_1 \geq 2$, and from finite induction, $v_n \geq 2$ for $1 \leq n \leq N$. So if k_n is computed from (5.1) in which b_n is given by (1.3), c_n is specified as in (4.5), and $\lambda_2 = 2 - 4/(4N+1)$, then k_n will satisfy

$$k_n^2 = c_n(k_{n-1} + k_n)(k_n + k_{n+1})/b_n b_{n-1} \quad (5.12)$$

for $1 \leq n \leq N-1$ and will be positive. Use these quantities in (2.3) to compute m_n for $1 \leq n \leq N-1$. The m_n so calculated will all be positive; and (2.4) will be satisfied by virtue of (5.12). By Theorem 3.5,

$$\phi_n(\omega^2) = D_n B_n^{(a,2)}(\mu\omega^2 + \nu) \quad \text{for} \quad 0 \leq n \leq N,$$

where

$$\begin{aligned} a &= -(4N+1)/2, \\ \mu &= 32(2N^3+1)/(4N+1)(4N-3)b_0, \\ \nu &= 4(16N^3 + 4N + 5)/(4N-3)(4N+1), \end{aligned}$$

and the polynomials are of the classical generalized Bessel type.

An appreciable number of "closed-form" constructions for the Laguerre and Jacobi cases are known. Some of them are now presented. In the Laguerre case, a constructive scheme that furnishes examples other than those to be given is also available (Ref. 1, Chap. 5); its technique is similar to the one already elaborated in the Hermite and Bessel cases.

To begin with, an Nth-order spring–mass configuration in which $m_0 > 0$, $k_1 > 0$, $k_n = nk_1$ for $0 \leq n \leq N$, and $m_n = m_0$ for $1 \leq n \leq N-1$ furnishes an example of an Nth-order Laguerre system in which $k_0 = 0$ (the left end of the configuration is free). By Theorem 3.3, the characteristic polynomials of this system are $\phi_n(\omega^2) = D_n L_n^0(m_0\omega^2/k_1)$ for $0 \leq n \leq N$.

As an example of a Laguerre system in which $k_0 > 0$, choose $k_0 > 0$, $m_0 > 0$, $k_n = k_0$ for $1 \leq n \leq N$, and $m_n = m_0/(n+1)$ for $1 \leq n \leq N-1$. In this case $\phi_n(\omega^2) = D_n L_n^1(m_0\omega^2/k_0)$ for $0 \leq n \leq N$. The construction can be generalized as follows: Choose $k_0 > 0$, $m_0 > 0$, $a > 0$,

$$k_n = n!\, k_0/a(a+1)\cdots(a+n-1)$$

for $1 \leq n \leq N$, and $m_n = n!\, m_0/(a+1)\cdots(a+n)$ for $1 \leq n \leq N-1$. Then each k_n and m_n is positive, and all conditions of Theorem 3.5 are satisfied. So $\phi_n(\omega^2) = D_n L_n^a(am_0\omega^2/k_0)$ for $0 \leq n \leq N$.

As an example of a family of Nth-order Jacobi-type systems in which $k_0 > 0$, first choose $r > 0$, $k_0 > 0$, and $m_0 > 0$. Then set $k_n = k_0 r^n$ for $1 \leq n \leq N$ and $m_n = m_0 r^n$ for $1 \leq n \leq N-1$. By Theorem 3.7,

$$\phi_n(\omega^2) = D_n P_n^{(a,b)}[1 - 2(\mu\omega^2 + \nu)], \quad \text{for} \quad 0 \leq n \leq N,$$

where $a = b = \frac{1}{2}$, $\mu = m_0/4k_0 r^{\frac{1}{2}}$, and

$$\nu = -(r^{\frac{1}{2}} - 1)^2/4r^{\frac{1}{2}}.$$

It follows that

$$\phi_n(\omega^2) = (-1)^n D_n V_n[2(\mu\omega^2 + \nu) - 1],$$

for $0 \leq n \leq N$, where V_n is the Tchebycheff polynomial of degree n of the second kind. Note that the simple case in which all spring constants are equal and all masses are equal is included within this family. Such a model is sometimes appropriate for structure theory of homogeneous media. In this case

$$\phi_n(\omega^2) = (-1)^n D_n V_n(-1 + m_0\omega^2/2k_0),$$

for $0 \leq n \leq N$.

An example in which $k_0 = 0$ is furnished by the following. Choose $m_0 > 0$ and $k_1 > 0$. Then set $k_n = nk_1$ for $0 \leq n \leq N$ and $m_n = (2n + 1)m_0$ for $1 \leq n \leq N - 1$. From Theorem 3.7,

$$\phi_n(\omega^2) = (-1)^n D_n P_n(-1 + m_0\omega^2/k_1),$$

for $0 \leq n \leq N$, where $P_n \equiv P_n^{(0,0)}$ is the Legendre polynomial of degree n.

As a final example of a Jacobi system, let $m_0 > 0$, $k_n = m_0/2(2n + 1)$ for $0 \leq n \leq N$, and $m_n = m_0/(n + 1)$ for $1 \leq n \leq N - 1$. Then

$$\phi_n(\omega^2) = (-1)^n D_n P_n^{(0,1)}(2\omega^2 - 1)$$

for $0 \leq n \leq N$.

6. THE INFINITE-ORDER CASE

The remainder of the answer to question (iii) is provided in this section. Specifically, that portion of the question which relates to question (ii) is developed. For the infinite-order case, the following three theorems show that of the four possible kinds, only Jacobi- and Laguerre-type systems can ever be generated; and the latter type can occur only if relatively stringent conditions on m_n and k_n are satisfied.

Theorem 6.1: For a given set of values m_0, m_1, k_0, k_1, k_2, it is impossible, by successively adding springs and masses as shown in Fig. 1, to construct an infinite-order system of harmonic oscillators such that $\phi_n(\omega^2) = D_n H_n(\mu\omega^2 + \nu)$ for every nonnegative integer n.

Proof: Suppose the contrary. Then from Eqs. (2.3), (2.4), and (4.1) and (4.2) in which $b_1 = b_0$,

$$(k_n + k_{n+1})/m_n = (k_0 + k_1)/m_0, \tag{6.1}$$

$$k_n^2/m_n m_{n-1} = nk_1^2/m_1 m_0, \quad \text{for} \quad n \geq 1. \tag{6.2}$$

From (6.2) it follows that

$$k_n^2/m_n^2 = nm_{n-1}k_1^2/m_0 m_1 m_n,$$
$$k_{n+1}^2/m_{n+1}^2 = (n + 1)m_{n+1}k_1^2/m_0 m_1 m_n;$$

and when these expressions are inserted into (6.1), the result can be written as

$$(k_0 + k_1)/m_0 n^{\frac{1}{2}} = k_1[(m_n/m_{n-1})^{-\frac{1}{2}} + (1 + 1/n)^{\frac{1}{2}}(m_{n+1}/m_n)^{\frac{1}{2}}]/(m_0 m_1)^{\frac{1}{2}}. \tag{6.3}$$

Suppose $\lim_{n\to\infty} m_{n+1}/m_n = L^2 > 0$. Then, when the limits of both sides of (6.3) are taken, the result is $0 = k_1(L + 1/L)/(m_0 m_1)^{\frac{1}{2}}$, a contradiction. If

$$\lim_{n\to\infty} \frac{m_{n+1}}{m_n} = 0$$

or if this limit does not exist, the left side of (6.3) still has limit zero, but the right side has no limit—another contradiction.

Theorem 6.2: For a given set of values m_0, m_1, k_0, k_1, k_2, it is impossible, by successively adding springs and masses as shown in Fig. 1, to construct an infinite-order system such that $\phi_n(\omega^2) = D_n B_n^{(a,b)}(\mu\omega^2 + \nu)$ for every nonnegative integer n.

Proof: Suppose otherwise. Then $k_n^2/m_n m_{n-1} \equiv c_n > 0$ for $n \geq 1$ and $(k_n + k_{n+1})/m_n \equiv -b_n > 0$ for $n \geq 0$. From Theorem 4.3, $2 - 2/(2N - 3) < \lambda_2 < 2$ for every integer $N \geq 3$, a contradiction.

Theorem 6.3: For a given set of values m_0, m_1, k_0, k_1, k_2, it is possible, by successively adding springs and masses as shown in Fig. 1, to construct an infinite-order system of harmonic oscillators such that $\phi_n(\omega^2) = D_n L_n^a(\mu\omega^2 + \nu)$ for every nonnegative integer n only if

$$\lim_{n\to\infty} \frac{m_{n+1}}{m_n} = 1,$$

$$\lim_{n\to\infty} \frac{k_{n+1}}{k_n} = 1,$$

and

$$\lim_{n\to\infty} \frac{k_n}{nm_{n-1}} = \frac{(k_2 + k_1)}{2m_1} - \frac{(k_1 + k_0)}{2m_0}.$$

Proof: Suppose first that an infinite-order Laguerre-type system has been constructed but

$$\lim_{n\to\infty} \frac{m_{n+1}}{m_n} = 1$$

does not hold. Then $c_n > 0$ for $n \geq 1$ so that the expression for b_n in (2.3) can be rewritten as

$$b_n/n = -(c_n m_{n-1}/n^2 m_n)^{\frac{1}{2}} - (c_{n+1}m_n/(n + 1)^2 m_{n+1})^{\frac{1}{2}}(n + 1)/n, \tag{6.4}$$

for $n \geq 1$. From Eqs. (4.1), (4.2), and Theorem 4.2,

$$\lim_{n\to\infty} \frac{b_n}{n} = b_1 - b_0,$$

$$\lim_{n\to\infty} \frac{c_n}{n^2} = \frac{(b_1 - b_0)^2}{4},$$

and $b_1 < b_0$. Suppose that

$$\lim_{n\to\infty} \frac{m_{n+1}}{m_n} = L^2,$$

where $L > 0$ and $L \neq 1$. Then, as $n \to \infty$, (6.4) yields

$$b_1 - b_0 = \frac{(b_1 - b_0)}{2L} + \frac{(b_1 - b_0)L}{2},$$

which implies $L = 1$, a contradiction. If $L = 0$ or $L = +\infty$, the right side of (6.4) has no limit—another contradiction. Finally, suppose that the sequence $\{m_{n+1}/m_n\}$ of positive terms has no limit but does have a finite limit inferior (an infinite limit inferior implies $L = +\infty$, a case already considered). Let $A = \liminf (m_n/m_{n-1})^{\frac{1}{2}}$. Then $A \geq 0$, and there exists a subsequence $\{(m_{n_k}/m_{n_k-1})^{\frac{1}{2}}\}$ with limit A. Equation (6.4) must hold for all terms of this subsequence; hence, as $n_k \to \infty$, (6.4) yields

$$2 = \frac{1}{A} + \lim_{n_k\to\infty} \left(\frac{m_{n_k+1}}{m_{n_k}}\right)^{\frac{1}{2}} \geq A + \frac{1}{A}, \qquad (6.5)$$

provided that $A \neq 0$. If $A = 0$, the same contradiction arises as was noted above under the assumption that $L = 0$. From (6.5) it follows that $A = 1$. Now let $B = \limsup (m_n/m_{n-1})^{\frac{1}{2}}$. Then $B \geq 1$. Denote a subsequence which converges to B by $\{(m_{n_j+1}/m_{n_j})^{\frac{1}{2}}\}$. Equation (6.4) must hold for the terms of this subsequence also. So

$$2 = \left[\lim_{n_j\to\infty} \left(\frac{m_{n_j}}{m_{n_j-1}}\right)^{\frac{1}{2}}\right]^{-1} + B \geq B + \frac{1}{B}, \qquad (6.6)$$

provided that B is finite. In this case $B = 1$, so that $A = B$, which contradicts the assumption that $\{m_{n+1}/m_n\}$ has no limit. If B is not finite, the same contradiction arises from (6.4) (with the terms of the subsequence which converges to B inserted) as was noted under the assumption above that $L = +\infty$.

At this stage it has been established that any infinite-order Laguerre-type system will have

$$\lim_{n\to\infty} \frac{m_{n+1}}{m_n} = 1.$$

This fact makes it easy to complete the proof.

From (2.4), in which c_n is given by (4.2) for $n \geq 1$, there follows

$$\lim_{n\to\infty} \frac{k_{n+1}^2}{k_n^2} = \lim_{n\to\infty} \left(\frac{m_{n+1}}{m_n} \cdot \frac{m_n}{m_{n-1}} \cdot \frac{c_{n+1}}{c_n}\right) = 1, \qquad (6.7)$$

$$\lim_{n\to\infty} \left(\frac{k_n}{nm_{n-1}}\right)^2 = \lim_{n\to\infty} \left(\frac{m_n}{m_{n-1}} \cdot \frac{c_n}{n^2}\right) = \tfrac{1}{4}(b_1 - b_0)^2. \qquad (6.8)$$

Since $b_1 < b_0$ and since $k_n/nm_{n-1} > 0$, $k_{n+1}/k_n > 0$ for $n \geq 1$, it follows that $\lim_{n\to\infty} k_{n+1}/k_n = 1$ and $\lim_{n\to\infty} k_n/nm_{n-1} = (b_0 - b_1)/2$. This completes the proof.

To furnish constructions of either infinite-order Laguerre- or Jacobi-type systems, one need only extend the range of index n to all nonnegative integers in each of the examples presented in Sec. 5. Unfortunately, this procedure will not convert *all* finite order Laguerre- or Jacobi-type systems to the corresponding infinite-order ones. In particular, a large class of systems is known (Ref. 1, Chap. 5) having the following property: For each preassigned integer $N \geq 3$, formulas for k_n and m_n can be given which provide a Laguerre-type system for any positive $n \leq N$, but fail to do so for some $n > N$.

As a final point, note that Theorem 4.4 implies that any infinite-order Jacobi-type system will have $\lambda_2 > 2$. Consequently, by Remark 4.2, generalized Jacobi polynomials in the infinite case cannot occur; the characteristic polynomials generated will be of the classical Jacobi type.

ACKNOWLEDGMENTS

The authors wish to acknowledge the many helpful suggestions of Dr. M. B. Sledd, Dr. D. V. Ho, and Dr. W. R. Smythe of the School of Mathematics, Georgia Institute of Technology. Without their comments, several results of this paper would not have appeared here.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Kernel Integral Formulas for the Canonical Commutation Relations of Quantum Fields.* I. Representations with Cyclic Field

GERHARD C. HEGERFELDT†
Institut für Theoretische Physik, Universität Marburg, Germany

(Received 25 November 1968)

We investigate the kernel or group integral for the canonical commutation relations introduced by Klauder and McKenna and its generalizations. For the finite case the kernel integral formula has been proven by means of the Schrödinger representation. Motivated by the close similarity of the Schrödinger representation to the form of a general representation with cyclic field, we examine these representations with respect to kernel integral formulas. A general criterion is derived in which the dimensionality of the test function space does not enter, i.e., it is independent of the number of degrees of freedom. In this way the finite and infinite case can be treated on equal footing. The criterion contains as special cases the kernel integral formulas of Klauder and McKenna for finitely many degrees of freedom and for direct- (or tensor-) product representations of fields. For partial tensor-product representations we obtain a somewhat modified formula. After these applications, a considerably sharpened form of the criterion is derived in which only the vacuum expectation functional enters. Under a certain cyclicity assumption it is shown that the validity of a kernel integral for just some cyclic vector implies its validity for all vectors. It is further shown that the basis-independent integral defined by a supremum over all bases of the test function space $\mathfrak{V}$ can be replaced by an ordinary limit over a kind of diagonal sequence through finite-dimensional subspaces of $\mathfrak{V}$. In the last section a representation is constructed which possesses a cyclic field but does not fulfil a kernel integral formula; this is an instructive illustration of a general theorem to be proved in II of this series of papers.

1. INTRODUCTION

In a quantum field theory which is based on the canonical (equal-time) commutation relations between the field Φ and the conjugate field Π, one has to look for a realization of the fields as operators in a Hilbert space. The operators have to satisfy

$$[\Phi(\mathbf{x}), \Pi(\mathbf{x}')] = i\delta^{(3)}(\mathbf{x} - \mathbf{x}'), \qquad (1.1)$$

with the other commutators vanishing. This problem is completely analogous to that of quantum mechanics where one starts with $[Q, P] = i$. There one knows that an irreducible representation is, up to unitary equivalence, uniquely given by the Schrödinger representation if one makes certain assumptions on the domains of definition of the operators. In quantum field theory the situation is completely different. Here uncountably many inequivalent irreducible representations[1] exist, so that the correct choice of a representation for physical applications becomes an important problem.

Mostly one takes the Fock representation, as for instance in the conventional formulation of quantum electrodynamics. However, one immediately encounters a fundamental difficulty in the form of Haag's theorem.[2] The Fock representation describes in a satisfactory manner the free field; but, according to Haag's theorem, the free field and interacting field are inequivalent to each other, so that, for instance, the interaction picture does not exist in a well-defined way. Some of the divergences which appear in the usual theory may well be connected to this, and the correct choice of the representation may become decisive. There exist exactly soluble field-theoretic models[3] which do not employ the Fock representation and for which one obtains always incorrect results with the usual perturbation and Green's function methods.[4]

Unfortunately, the representations of the canonical commutation relations (CCR) possess a rather complicated structure, and one still has no complete classification of all representations up to unitary equivalence; only for a very special class has this been carried through.[5] One does have a number of general existence theorems, and one can characterize the representations either by measures[6] or by vacuum expectation values of the fields.[7] But in general it is impossible to construct these measures explicitly. The connection between the measures and the vacuum expectation values is, therefore, more of theoretical interest. Both methods are not very appropriate for constructive realizations of representations useful

* Based on a part of the author's Habilitationsschrift, "*Aspekte der kanonischen Vertauschungsrelationen für Quantenfelder*," University of Marburg, 1968. Paper II, with the subtitle "Irreducible Representations," will appear shortly in this same journal.

† Address from October 1969: Institut für Theoretische Physik der Universität, Göttingen, Germany.

[1] For an early reference see L. Gårding and A. Wightman, Proc. Natl. Acad. Sci. US **40**, 622 (1954).

[2] R. Haag, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. **29**, 12 (1955).

[3] J. R. Klauder, J. Math. Phys. **6**, 1666 (1965).

[4] H. D. I. Abarbanel, J. R. Klauder, and J. G. Taylor, Phys. Rev. **152**, 1198 (1966).

[5] J. R. Klauder, J. McKenna, and E. J. Woods, J. Math. Phys. **7**, 822 (1966).

[6] See Ref. 1 and I. S. Lew, Ph.D. thesis, Princeton University, 1960 (unpublished).

[7] H. Araki, J. Math. Phys. **1**, 492 (1960).

for practical applications. In some cases[8] one can employ a generalization of the method used in the Fock representation.

In this context some new results on irreducible representations of the commutation relations

$$[Q_j, P_k] = i\delta_{jk}$$

for n degrees of freedom are interesting. It has been shown[9] that, by means of the so-called reproducing kernel, the operators Q_j, P_j can be realized in spaces of continuous functions of $2n$ variables, in contrast to the Schrödinger representation, where one needs equivalence classes of square-integrable functions of n variables. The scalar product in this space is defined by integration over the $2n$ variables, a kind of group integral. The Schrödinger representation for finitely many degrees of freedom is quite well known and, therefore, the importance of such a realization lies probably mainly in its application to coherence properties in quantum optics.[10]

For infinitely many degrees of freedom, that is, for Bose fields, an analogous property would be of great theoretical and practical interest. But one immediately encounters the difficulty that for $n \to \infty$ one deals with continuous functions of an infinite number of variables, and it is unclear how to define the integration for the scalar product in this case. For a special class of representations, the tensor- or direct-product representations, one has succeeded in constructing such a realization by continuous functions where the scalar product is now given by a limit over ordinary finite-dimensional integrations with the number of integration variables tending towards infinity.[11] The general case is still unsolved.

Realizations in spaces of continuous functions are always possible; the main problem, however, is whether one can obtain the scalar product in this space by ordinary integration. It is easy to reduce this question to a property of the kernel or of the vacuum expectation value of the representation. The kernel has to satisfy a certain integral formula; a kind of generalized convolution of the kernel with itself has to reproduce the kernel. Together with other basic prerequisites, we explain this in more detail in Sec. 2. We discuss in particular how the integral for finitely many degrees of freedom can be carried over to fields. There, three possibilities arise. One can introduce an orthonormal basis in the space of test functions, integrate over the first n degrees of freedom, and let n go towards infinity. One can, if this limit does not exist, consider norms and take a limit superior. Or one can consider the supremum over all bases, so that the integral becomes basis-independent.

The question, if and where such kernel integral formulas exist, is investigated in this paper. The proof for the case of a finite number of degrees of freedom makes use of the Schrödinger representation in an essential way. Since for an infinite number of degrees of freedom there is a host of inequivalent representations, a direct carrying over of the proof is impossible.

Besides irreducibility the Schrödinger representation possesses a further property. The operators Q or Q_i, respectively, are cyclic, i.e., there exists a vector φ_0 in the Hilbert space $\mathfrak{H}$ such that the linear combinations of vectors of the form $Q^N\varphi_0$ lie dense in $\mathfrak{H}$. In the usual realization of $\mathfrak{H}$ as the space of square-integrable functions and of Q as multiplication by x, one can take for φ_0 every function which differs from zero almost everywhere. Conversely, every representation with a cyclic Q is irreducible and hence equivalent to the Schrödinger representation. In the infinite case the analogous property does not hold. There are irreducible representations for which the field Φ is not cyclic, and there are also representations with the field Φ cyclic which are not irreducible.[7]

If there exist any kernel integral formulas for fields, one immediately encounters the interesting question of which of the two properties is carried over—irreducibility or field cyclicity. At first sight, the form of the Schrödinger representation points to field cyclicity because it closely resembles the general form of a representation with cyclic field. In Paper I, therefore, we investigate these representations with respect to kernel integral formulas.

The general form[12] of these representations (cf. Sec. 3), which also holds in the finite case, allows a simultaneous investigation of finitely many and of infinitely many degrees of freedom (fields) without using the special nature of the Schrödinger representation. In Sec. 4 we derive a general criterion for the existence of kernel integral formulas in representations with cyclic field operator. After simple applications to tensor-product and partial tensor-product representations, the criterion is sharpened considerably in Sec. 6 such that only vacuum expectation values enter. In Sec. 7 we finally show by a simple example that not every representation with cyclic field can satisfy a kernel integral formula. This will lead us in Paper II to the investigation of irreducible representations.

[8] H. Araki and E. J. Woods, J. Math. Phys. **4**, 637 (1963).
[9] J. McKenna and J. R. Klauder, J. Math. Phys. **5**, 878 (1964).
[10] J. R. Klauder, in *Brandeis Lectures 1967* (Gordon and Breach, Science Publ., New York, to be published); J. R. Klauder, J. McKenna, and D. G Currie, J. Math. Phys. **6**, 734 (1965).
[11] J. R. Klauder and J. McKenna, J. Math. Phys. **6**, 68 (1965).
[12] The present paper seems to be the first somewhat more practical application of this.

2. PRELIMINARIES: KERNEL INTEGRAL FORMULAS

In order to give the CCR in (1.1) a mathematically precise meaning, one has, in view of the δ function, to consider the fields as operator-valued distributions. One therefore replaces $\Phi(\mathbf{x})$, $\Pi(\mathbf{x})$ by $\Phi(f)$, $\Pi(g)$, where f and g lie in a subspace $\mathfrak{U}$ of all real square-integrable functions on R^3 and where $\Phi(f)$, $\Pi(g)$ can be considered heuristically as "smeared" field operators:

$$\Phi(f) = \int \Phi(\mathbf{x}) f(\mathbf{x})\, d^3x, \quad \Pi(g) = \int \Pi(\mathbf{x}) g(\mathbf{x})\, d^3x. \tag{2.1}$$

By formal calculation one obtains

$$\begin{aligned} [\Phi(f_1), \Phi(f_2)] &= [\Pi(g_1), \Pi(g_2)] = 0, \\ [\Phi(f), \Pi(g)] &= i(f, g), \end{aligned} \tag{2.2}$$

where

$$(f, g) = \int f(\mathbf{x}) g(\mathbf{x})\, d^3x.$$

Because of Eq. (2.1), one demands

$$\begin{aligned} \Phi(f_1 + f_2) &= \Phi(f_1) + \Phi(f_2), \\ \Pi(g_1 + g_2) &= \Pi(g_1) + \Pi(g_2). \end{aligned} \tag{2.3}$$

$\mathfrak{U}$ is called the test function space. Because the operators in Eq. (2.2) are unbounded, one still has to specify their domain of definition. In order to avoid these complications, one replaces $\Phi(f)$ and $\Pi(g)$ by the Weyl operators $U(f)$ and $V(g)$, whose connection with the fields is formally given by

$$\begin{aligned} U(f) &= e^{i\Phi(f)}, \\ V(g) &= e^{i\Pi(g)}. \end{aligned} \tag{2.4}$$

Formal application of Eqs. (2.2) and (2.3) yields

$$\begin{aligned} U(f_1)U(f_2) &= U(f_1 + f_2), \\ V(g_1)V(g_2) &= V(g_1 + g_2), \\ V(g)U(f) &= e^{i(f,g)}U(f)V(g). \end{aligned} \tag{2.5}$$

The postulated unitarity of $U(f)$ and $V(g)$ implies

$$\begin{aligned} U(0) &= V(0) = \mathbf{1}, \\ U(f)^* &= U(-f), \\ V(f)^* &= V(-f). \end{aligned} \tag{2.6}$$

Relations (2.5) and (2.6) are usually taken as a starting point for rigorous mathematical investigations of the CCR. It should be noted, however, that there are more representations for the fields than for the Weyl operators because the unitary operators in (2.4) need not exist in a well-defined way; and even if they exist, Eq. (2.5) need not hold. Conversely, one can always obtain the field operators from $U(f)$ and $V(g)$ by Stone's theorem if one imposes appropriate continuity conditions. The preference for the Weyl operators over the fields has to be justified by physical arguments. In quantum mechanics the integrability of the operators P and Q, i.e., the existence of the unitary operators satisfying relations analogous to Eqs. (2.4) and (2.5), is closely related to Galilei invariance.

As a further requirement for a representation of the CCR, one assumes weak continuity for each degree of freedom, or, more precisely, for each f and g in $\mathfrak{U}$ the operators $U(\lambda f)$ and $V(\lambda g)$ are assumed to be weakly continuous in λ. Because of unitarity, this implies strong continuity. In addition, one has by Eq. (2.5) for fixed $f_1, \cdots, f_n$ and $g_1, \cdots, g_m$ that

$$U\left(\sum_1^n \lambda_i f_i\right) \quad \text{and} \quad V\left(\sum_1^m \lambda_i g_i\right)$$

are (weakly and strongly) continuous in λ_i. As an abbreviation we put

$$U(f, g) \equiv U(f) \cdot V(g). \tag{2.7}$$

Definition 2.1: By a representation of the CCR with test function space $\mathfrak{U}$ we mean a family of operators $U(f)$, $V(g)$ with $f, g \in \mathfrak{U}$, which fulfill Eqs. (2.5) and (2.6) and for which $U(\lambda f)$, $V(\lambda g)$ depend continuously on λ.

The CCR are closely connected with a group G whose elements are triplets $\mathfrak{g} = (\alpha; f, g)$, where α is a complex number of modulus 1 and where f and g are in $\mathfrak{U}$. The group relation is

$$\mathfrak{g}_1\mathfrak{g}_2 = (e^{i(f_2,g_1)}\alpha_1\alpha_2; f_1 + f_2, g_1 + g_2). \tag{2.8}$$

Therefore every representation of the CCR is a unitary representation of the group G where $(\alpha; 0, 0)$ is mapped onto $\alpha \cdot \mathbf{1}$.

A representation of the CCR is called cyclic if there exists a vector φ_0 in $\mathfrak{H}$ such that the finite linear combinations of vectors of the form $U(f, g)\varphi_0$ are dense in $\mathfrak{H}$. Every unitary representation is a direct sum of cyclic representations; for a nonseparable Hilbert space $\mathfrak{H}$ the sum may be uncountable. With every cyclic representation and cyclic unit vector one can associate the expectation value

$$E(f, g) \equiv \langle \varphi_0, U(f, g)\varphi_0 \rangle. \tag{2.9}$$

This is a function on $\mathfrak{U} \times \mathfrak{U}$, and, because in physical applications one often assumes the vacuum to be cyclic, $E(f, g)$ will be called *vacuum functional.*

Let f_i, $g_i \in \mathfrak{U}$ and let λ_i be complex numbers, $i = 1, \cdots, n$. Then

$$0 \leq \left\| \sum_1^n \lambda_i U(f_i, g_i)\varphi_0 \right\|^2$$

implies, by Eq. (2.5),

$$\sum_{i,j} \lambda_i \bar{\lambda}_j e^{-i(f_i - f_j, g_j)} E(f_i - f_j, g_i - g_j) \geq 0. \quad (2.10)$$

One further has

$$\overline{E(f, g)} = E(-f, -g) e^{i(f,g)}. \quad (2.11)$$

Araki[7] has shown that every cyclic representation of the CCR can be characterized by its vacuum functional:

Theorem 2.1: The functional $E(f, g)$ determines a cyclic representation up to unitary equivalence. To every functional on $\mathfrak{U} \times \mathfrak{U}$ which fulfills Eqs. (2.10) and (2.11) there exists a cyclic representation. For the continuity of $U(f)$ and $V(g)$ in some topology of $\mathfrak{U}$, it is necessary and sufficient that $E(f, g)$ is continuous in f and g separately.

To prove the unitary equivalence of two representations $U(f, g)$, $\hat{U}(f, g)$ with cyclic vectors φ_0, $\hat{\varphi}_0$ and with $\langle \varphi_0, U(f, g)\varphi_0 \rangle = \langle \hat{\varphi}_0, \hat{U}(f, g)\hat{\varphi}_0 \rangle$, one maps the vectors $\sum \lambda_i U(f_i, g_i)\varphi_0$ onto $\sum \lambda_i \hat{U}(f_i, g_i)\hat{\varphi}_0$. This mapping is isometric by the same reasoning which led to Eq. (2.10). The proof that to every vacuum functional there exists a representation was carried out by Araki[7] with the help of self-adjoint algebras. However, if one starts from the group G in Eq. (2.8), this part of the theorem is an immediate consequence of a simple result about positive group functionals.[13] The construction outlined further below will also imply this.

The kernel $K(f, g; f', g')$ of a cyclic representation is connected in a simple manner with the vacuum functional. Let φ_0 be a cyclic unit vector, and put

$$|f, g\rangle \equiv U(f, g)\varphi_0, \quad (2.12)$$

$$K(f, g; f', g') \equiv \langle f, g \,|\, f', g' \rangle = \langle U(f, g)\varphi_0, U(f', g')\varphi_0 \rangle. \quad (2.13)$$

In the same way as Eqs. (2.10) and (2.11) one obtains

$$\sum \bar{\lambda}_j \lambda_i K(f_j, g_j; f_i, g_i) \geq 0, \quad (2.14)$$

$$\overline{K(f, g; f', g')} = K(f', g'; f, g), \quad (2.15)$$

$$K(f, g; f, g) = 1, \quad (2.16)$$

$$K(f, g; f', g') = e^{i(f - f', g)} K(0, 0; f' - f, g' - g), \quad (2.17)$$

$$K(0, 0; f, g) = E(f, g). \quad (2.18)$$

The linear combinations of the vectors $|f, g\rangle$ in Eq. (2.12) are dense in $\mathfrak{K}$ because φ_0 is cyclic by assumption. Every $\varphi \in \mathfrak{K}$ is therefore uniquely determined by the function

$$\varphi(f, g) \equiv \langle f, g \,|\, \varphi \rangle \quad (2.19)$$

on $\mathfrak{U} \times \mathfrak{U}$. It follows from the assumed continuity properties of the representation that $\varphi(\sum_1^n \lambda_i f_i, g)$ is continuous in λ_i for fixed f_i, g, and similarly for $\varphi(f, \sum \lambda_i g_i)$. If one imposes stronger continuity conditions, $\varphi(f, g)$ becomes continuous in an analogous way. According to (2.5), the operators $U(f)$, $V(g)$ act on $\varphi(f, g)$ in the following way:

$$(U(f')\varphi)(f, g) = \varphi(f - f', g),$$
$$(V(g')\varphi)(f, g) = e^{i(f, g')}\varphi(f, g - g'). \quad (2.20)$$

The totality of all such functions $\varphi(f, g)$ is a subspace of the space of all continuous and, because of $|\langle f, g \,|\, \varphi \rangle| \leq \|\varphi\|$, bounded functions on $\mathfrak{U} \times \mathfrak{U}$. Here, continuous is meant in the above sense. This subspace is determined by the kernel, as is shown by the following construction of a representation by means of the kernel.[14]

Let $K(f, g; f', g')$ be a function on $\mathfrak{U} \times \mathfrak{U} \times \mathfrak{U} \times \mathfrak{U}$ satisfying Eqs. (2.14)–(2.17). Let $\mathfrak{L}$ be the set of all functions on $\mathfrak{U} \times \mathfrak{U}$ of the form

$$\varphi(f, g) = \sum_1^n \lambda_i K(f, g; f_i, g_i), \quad n = 1, 2, \cdots, \quad (2.21)$$

where the λ_i run through the complex numbers and f_i, g_i through $\mathfrak{U}$. Let

$$\varphi'(f, g) = \sum_1^m \lambda'_j K(f, g; f'_j, g'_j).$$

One defines a positive-definite bilinear Hermitian form (φ, φ') on $\mathfrak{L}$ by

$$(\varphi, \varphi') \equiv \sum_{i=1}^n \sum_{j=1}^m \bar{\lambda}_i \lambda'_j K(f_i, g_i; f'_j, g'_j). \quad (2.22)$$

By Eq. (2.14) one has $(\varphi, \varphi) \geq 0$; in particular,

$$(\varphi, \varphi) = \sum_{i,j} \bar{\lambda}_i \lambda_j K(f_i, g_i; f_j, g_j) = \sum_i \bar{\lambda}_i \varphi(f_i, g_i). \quad (2.23)$$

With $\varphi'(f, g) = K(f, g; f', g')$, from (2.22), in a similar way, one obtains

$$\varphi(f', g') = (\varphi', \varphi) = (K(f, g; f', g'), \varphi(f, g)), \quad (2.24)$$

[13] M. A. Neumark, *Normierte Algebren* (VEB Deutsches Verlag der Wissenschaften, Berlin, 1959), p. 401, Theorem 1.

[14] N. Aronzajn, Trans. Am. Math. Soc. **68**, 337 (1950); cf. also Ref. 9.

and from this, by Schwarz's inequality and Eq. (2.23), we get

$$|\varphi(f', g')|^2 \leq (\varphi, \varphi) \cdot (\varphi', \varphi') = (\varphi, \varphi) \cdot K(f', g'; f', g') = (\varphi, \varphi). \tag{2.25}$$

Therefore $(\varphi, \varphi) = 0$ implies the identical vanishing of $\varphi(f, g)$. Thus one has in $\mathfrak{L}$ a scalar product and a norm $\|\varphi\| = (\varphi, \varphi)^{\frac{1}{2}}$, with respect to which $\mathfrak{L}$ can be completed to a Hilbert space. Let $\varphi_n(f, g)$ be a Cauchy sequence in $\mathfrak{L}$, $\|\varphi_n - \varphi_m\| \to 0$, for $n, m \to \infty$. With $\varphi = \varphi_n - \varphi_m$ Eq. (2.25) then implies

$$|\varphi_n(f, g) - \varphi_m(f, g)| \leq \|\varphi_n - \varphi_m\|. \tag{2.26}$$

Thus the sequence of functions $\varphi_n(f, g)$ converges pointwise and uniformly to a function on $\mathfrak{U} \times \mathfrak{U}$ which has the same continuity properties as the kernel. The norm of the limit is as usual defined by $\lim \|\varphi_n\|$. Thus the closure of $\mathfrak{L}$ with respect to the norm in Eq. (2.23) consists of a Hilbert space of continuous functions determined by the kernel.

Now one defines linear operators $U(f')$, $V(g')$ in $\mathfrak{L}$ by Eq. (2.20). With Eq. (2.17) one shows at once that $\mathfrak{L}$ is invariant under these operators. In the same way one shows that the operators are unitary and satisfy the CCR. Their uniquely determined extension to the closure of $\mathfrak{L}$ therefore yields a representation of the CCR. Choosing $\varphi_0(f, g) = K(f, g; 0, 0)$, φ_0 becomes a cyclic vector; by (2.17) and (2.22), one obtains

$$(U(f', g')\varphi_0, U(f'', g'')\varphi_0) = K(f', g'; f'', g'').$$

For a given kernel one has thus constructed a representation by means of continuous functions, and one has simultaneously proved the second part of Theorem 2.1.

The scalar product in Eq. (2.22) is not very convenient because one has to express the functions in terms of the kernel. For infinitely many degrees of freedom, Klauder and McKenna[9] have shown that the scalar product can be obtained by integration if the representation is equivalent to the Schrödinger representation. Let $\mathfrak{U}$ be finite dimensional, and let $h_1, \cdots, h_n$ be an orthonormal basis of $\mathfrak{U}$. For any $f, g \in \mathfrak{U}$, one can write $f = \sum_1^n \alpha_i h_i$ and $g = \sum_1^n \beta_i h_i$. With the operators $U_j(\alpha_j) \equiv U(\alpha_j h_j)$ and $V_j(\beta_j) \equiv V(\beta_j h_j)$, $j = 1, \cdots, n$, one obtains the usual notation for a representation of the CCR with n degrees of freedom if one puts

$$U_j(\alpha_j) \equiv e^{i\alpha_j Q_j}, \quad V_j(\beta_j) \equiv e^{i\beta_j P_j}. \tag{2.27}$$

Let $d^n f$ denote the Lebesgue measure defined by the scalar product in $\mathfrak{U}$. With the above basis one can write $d^n f = d\alpha_1 \cdots d\alpha_n$. If the representation is irreducible, one can realize the U_j and V_j by the Schrödinger operators in the space L^2 of square-integrable functions on R^n:

$$(U_j(\alpha_j)\psi)(x_1, \cdots, x_n) = e^{ix_j\alpha_j}\psi(x_1, \cdots, x_n),$$
$$(V_j(\beta_j)\psi)(x_1, \cdots, x_n) = \psi(x_1, \cdots, x_j + \beta_j, \cdots, x_n). \tag{2.28}$$

By means of this realization Klauder and McKenna[9] have shown that for any normed $\varphi_0 \in L^2$, i.e., $\|\varphi_0\| = 1$, one has for all $\psi_1, \psi_2 \in \mathfrak{H}$,

$$\int d\alpha_1 \cdots d\alpha_n \, d\beta_1 \cdots d\beta_n/(2\pi)^n \times \langle \psi_1, \prod_1^n U_j(\alpha_j) \prod_1^n V_j(\beta_j)\varphi_0 \rangle \times \langle \prod_1^n U_j(\alpha_j) \prod_1^n V_j(\beta_j)\varphi_0, \psi_2 \rangle = \langle \psi_1, \psi_2 \rangle.$$

With (2.19) this can be rewritten as

$$\langle \psi_1, \psi_2 \rangle = \int_{\mathfrak{U}\times\mathfrak{U}} d^n f \, d^n g/(2\pi)^n \langle \psi_1, U(f, g)\varphi_0 \rangle \langle U(f, g)\varphi_0, \psi_2 \rangle = \int_{\mathfrak{U}\times\mathfrak{U}} d^n f \, d^n g/(2\pi)^n \bar{\psi}_1(f, g)\psi_2(f, g). \tag{2.29}$$

This can be viewed as a resolution of the unit operator:

$$\mathbf{1} = \int_{\mathfrak{U}\times\mathfrak{U}} d^n f \, d^n g/(2\pi)^n \, |f, g\rangle\langle f, g|.$$

Conversely, the representation is equivalent to the Schrödinger representation if (2.29) holds for all $\psi_1, \psi_2 \in \mathfrak{H}$. In Ref. 5 Eq. (2.29) was sharpened as follows:

Lemma 2.1: In the Schrödinger representation for n degrees of freedom, one has for all $\psi_1, \varphi_1, \varphi_2, \psi_2 \in \mathfrak{H}$

$$\int_{\mathfrak{U}\times\mathfrak{U}} d^n f \, d^n g/(2\pi)^n \langle \psi_1, U(f, g)\varphi_1 \rangle \langle U(f, g)\varphi_2, \psi_2 \rangle = \langle \psi_1, \psi_2 \rangle \langle \varphi_2, \varphi_1 \rangle. \tag{2.30}$$

For an arbitrary representation one has

$$\left| \int_{\mathfrak{U}\times\mathfrak{U}} d^n f \, d^n g/(2\pi)^n \langle \psi_1, U(f, g)\varphi_1 \rangle \langle U(f, g)\varphi_2, \psi_2 \rangle \right| \leq \|\psi_1\| \cdot \|\varphi_1\| \cdot \|\varphi_2\| \cdot \|\psi_2\|. \tag{2.31}$$

The last inequality implies that the functions $\varphi(f, g)$ are square integrable over $\mathfrak{U} \times \mathfrak{U}$. For fixed $f', g' \in \mathfrak{U}$, $K(f, g; f', g')$ is a particular $\varphi(f, g)$. Equation

(2.29) then implies the integral formula

$$\int_{\mathfrak{V}\times\mathfrak{V}} d^n f\, d^n g/(2\pi)^n K(f', g'; f, g) K(f, g; f'', g'') = K(f', g'; f'', g''). \quad (2.32)$$

Conversely, (2.29) follows from this for the φ_0 used in the definition of the kernel. Indeed, (2.32) is just (2.29) with $\psi_1 = |f', f'\rangle$ and $\psi_2 = |f'', g''\rangle$. Then (2.29) holds for all finite linear combinations of such vectors. Since φ_0 is assumed to be cyclic, (2.29) holds on a dense set of vectors ψ_1, ψ_2. The continuity properties contained in Eq. (2.31) then yield Eq. (2.29) for all $\psi_1, \psi_2 \in \mathcal{H}$. As will be shown in Part II, this implies the irreducibility of the representation and therefore the validity of (2.29) for any φ_0. One can also show directly[9] that a kernel satisfying (2.32) belongs to the Schrödinger representation.

Klauder and McKenna have succeeded in generalizing Eqs. (2.29) and (2.32) to tensor-product representations of the CCR for infinitely many degrees of freedom. There exists an orthonormal basis $h_1, h_2, \cdots$ of $\mathfrak{V}$ which enters in a natural way into the construction of tensor-product representations. Denote by W_n the subspace of $\mathfrak{V}$ spanned by the first n basis vectors. Then[5,11]

$$\lim_{n\to\infty} \int_{W_n\times W_n} d^n f\, d^n g/(2\pi)^n \langle \psi_1, U(f, g)\varphi_0\rangle \times \langle U(f, g)\varphi_0, \psi_2\rangle = \langle \psi_1, \psi_2\rangle \quad (2.33)$$

for all $\psi_1, \psi_2 \in \mathcal{H}$ and any normed $\varphi_0 \in \mathcal{H}$. Thus in the infinite case the integral over the parameter space $\mathfrak{V}$ has been replaced by a limit of integrals over finite-dimensional subspaces. Analogously to (2.32), one obtains for the kernel the integral formula

$$\lim_{n\to\infty} \int_{W_n\times W_n} d^n f\, d^n g/(2\pi)^n K(f', g'; f, g) \times K(f, g; f'', g'') = K(f', g'; f'', g''). \quad (2.34)$$

The question arises whether similar formulas also hold for other representations of the CCR. In the general case the limit in (2.33) need not exist, or its value might depend on the particular basis in $\mathfrak{V}$. For $\psi_1 = \psi_2$ the integrand in (2.33) is positive, and, according to (2.31), the integrals have a common bound so that at least the limit superior exists. Since one can express scalar products by norms, it would still be interesting if, instead of (2.33), one had

$$\overline{\lim_{n\to\infty}} \int_{W_n\times W_n} d^n f\, d^n g/(2\pi)^n |\langle \psi, U(f, g)\varphi_0\rangle|^2 = \|\psi\|^2 \quad (2.35)$$

for all $\psi \in \mathcal{H}$ and some unit vector φ_0. Since this integral depends on the particular basis $h_1, h_2, \cdots$, Klauder[15] has proposed to consider the supremum of the left-hand side of Eq. (2.35) over all bases. In this way one would get a basis independent integral. Let β be an index for the different bases $h_1^\beta, h_2^\beta, \cdots$ of $\mathfrak{V}$, and let W_n^β be the subspace spanned by $h_1^\beta, \cdots, h_n^\beta$. Then the question is whether

$$\sup_\beta \overline{\lim_n} \int_{W_n{}^\beta\times W_n{}^\beta} d^n f\, d^n g/(2\pi)^n |\langle \psi, U(f, g)\varphi_0\rangle|^2 = \|\psi\|^2 \quad (2.36)$$

holds for all $\psi \in \mathcal{H}$ and some unit vector φ_0. Of course this can hold only for a φ_0 which is cyclic with respect to $U(f, g)$, because the left-hand side is zero for any ψ orthogonal to the subspace of $\mathcal{H}$ generated by the vectors $U(f, g)\varphi_0$. Again one can replace (2.35) and (2.36) by expressions in which only the kernel enters. But these are now somewhat more complicated than (2.34) and not of interest here. Simpler expressions will be given in Paper II.

In a certain way the integrals in Eqs. (2.33)–(2.36) can be considered as *group integrals* over the parameter space $\mathfrak{V} \times \mathfrak{V}$ of the group G in (2.8). The resulting formulas will be called *kernel integral formulas*. We now turn to representations with a cyclic field, i.e., with $U(f)$ cyclic, and investigate them with respect to such formulas.

3. CYLINDER SETS

Every representation of the CCR with cyclic field can be realized by means of a measure μ in the space L_μ^2 of μ-square-integrable functions. Here μ is a measure on the dual space $\mathfrak{V}'$ of all linear functionals on $\mathfrak{V}$. For the following we need some properties of the measure and of the realization.

The space $\mathfrak{V}$ is a real linear vector space of finite or infinite dimension. Let $\mathfrak{V}'$ denote the totality of *all* real-valued linear functionals on $\mathfrak{V}$, i.e., not only those which are continuous in some topology of $\mathfrak{V}$. For instance, if $\mathfrak{V}$ consists of all square-integrable functions, the space of all continuous, i.e., bounded, functionals would be equal to $\mathfrak{V}$, while $\mathfrak{V}'$ is much larger. However, if $\mathfrak{V}$ is finite dimensional, $\mathfrak{V}$ is isomorphic to $\mathfrak{V}'$.

Let W be a finite-dimensional subspace of $\mathfrak{V}$, and let $W^0 \subset \mathfrak{V}'$ be the annihilator of W in $\mathfrak{V}'$, i.e., W^0 consists of all $F \in \mathfrak{V}'$ with

$$(F, f) = 0 \quad \text{for all} \quad f \in W. \quad (3.1)$$

Denote by η the natural homomorphism of $\mathfrak{V}'$ onto the factor space $\mathfrak{V}'/W^0$. The elements of $\mathfrak{V}'/W^0$ are the cosets $F + W^0$:

$$\eta: F \to F + W^0. \quad (3.2)$$

[15] J. R. Klauder, Ref. 10.

Definition 3.1: Let A be a subset of $\mathfrak{U}'/W^0$. The set $Z = \eta^{-1}(A)$, the inverse image of A in $\mathfrak{U}'$, is called a *cylinder set* with base A and generating subspace W.

We show that the factor space $\mathfrak{U}'/W^0$ can be considered as the dual space W' of W. Then W and $\mathfrak{U}'/W^0$ possess in particular equal (finite) dimension. By Eq. (3.1) all functionals which belong to the same coset coincide on W so that such a coset defines a linear functional on W. In this way one obtains every element of W'. For let $F_W \in W'$, and let $f_1, \cdots, f_N$ be some basis of W. This basis can be extended to a Hamel basis of $\mathfrak{U}$. Define a linear functional F on $\mathfrak{U}$ by $(F, f_i) \equiv (F_W, f_i)$ for $i = 1, \cdots, N$, and 0 for the rest of the Hamel basis. Then $F \in \mathfrak{U}'$, and F coincides on W with F_W.

Since there is a scalar product (f, g) in $\mathfrak{U}$, every element f of $\mathfrak{U}$ defines a linear functional F_f on $\mathfrak{U}$ by the equation

$$(F_f, g) \equiv (f, g) \quad \text{for all} \quad g \in \mathfrak{U}. \tag{3.3}$$

In this way one obtains an embedding of $\mathfrak{U}$ in $\mathfrak{U}'$. In the following we always identify F_f with f so that we can consider $\mathfrak{U}$ as a subspace of $\mathfrak{U}'$:

$$\mathfrak{U} \subset \mathfrak{U}'. \tag{3.4}$$

If W is a finite-dimensional subspace of $\mathfrak{U}$, one can identify W with W' by relation (3.3), so that, with the preceding remark, one can write

$$W = W' = \mathfrak{U}'/W^0. \tag{3.5}$$

Since with W also $\mathfrak{U}'/W^0$ is finite dimensional, one can take Borel sets for the base A in definition (3.1), which will always be done in the following. We now turn to cylinder measures.

Definition 3.2: A normed *cylinder measure* is a real-valued function $\mu(Z)$ on the family $\{Z\}$ of all cylinder sets Z belonging to finite-dimensional generating subspaces and Borel bases, with the following properties:

(1) $0 \leq \mu(Z) \leq 1$ for all Z;

(2) $\mu(\mathfrak{U}') = 1$;

(3) If $Z = \bigcup_1^\infty Z_i$ where all Z_i possess the same generating subspace and have pairwise-empty intersection, then

$$\mu(Z) = \sum_1^\infty \mu(Z_i).$$

The last condition does not mean that μ is countably additive on $\{Z\}$ because, in general, the generating subspace need not be the same. But one obviously has the following consequence.

Lemma 3.1: Every cylinder measure induces a countably additive measure $\tilde{\mu}$ on the Borel sets A of the factor space $\mathfrak{U}'/W^0$ by the definition

$$\tilde{\mu}(A) \equiv \mu(Z), \tag{3.6}$$

where Z is a cylinder set with Borel base A and generating subspace W.

If in addition μ is countably additive on $\{Z\}$, it can be extended to a countably additive measure on the σ-algebra B generated by $\{Z\}$.[16] The elements of B are called the *Borel sets of* $\mathfrak{U}'$.

The above results remain true if $\mathfrak{U}$ is a topological vector space, in particular, if $\mathfrak{U}$ is a nuclear space, like the space S of Schwarz, and if $\mathfrak{U}'$ is the space of continuous functionals on $\mathfrak{U}$. Some derivations, however, are different. Further details on cylinder sets and cylinder measures can be found in Ref. 17.

There exists an important connection between cylinder measures and representations of the CCR. Let $U(f, g), f, g \in \mathfrak{U}$, be a representation with cyclic field operator, and let φ_0 be a unit vector cyclic for $U(f)$. Then there exists[7] a normed countably additive measure μ on B, the Borel sets of $\mathfrak{U}'$, such that $U(f)$, $V(g)$ can be realized in the Hilbert space L^2_μ of μ-square-integrable functions[18] $\varphi(F)$ on $\mathfrak{U}'$ in the following way. The cyclic vector φ_0 corresponds to the function $\varphi_0(F) \equiv 1$, and

$$\begin{aligned} (U(f)\varphi)(F) &= e^{i(F,f)}\varphi(F), \\ (V(g)\varphi)(F) &= a_g(F)\varphi(F + g), \end{aligned} \tag{3.7}$$

with

$$a_g(F) = (V(g)\varphi_0)(F).$$

Due to the group property of the $V(g)$, the functions $a_g(F)$ fulfill the relation

$$a_g(F)a_{g'}(F + g) = a_{g+g'}(F). \tag{3.8}$$

Due to the unitarity of the representation, one has

$$d\mu(F + g) = |a_g(F)|^2 \, d\mu(F). \tag{3.9}$$

For $\mu(\Delta) = 0$, $\Delta \in B$, this implies $\mu(\Delta + g) = 0$ for all $g \in \mathfrak{U}$. This means that μ is quasi-invariant.

The space $\mathfrak{U}'$ is rather large, and one would like to replace it (through suitable continuity conditions) by a smaller one. In general, this is not possible. However, if $\mathfrak{U}$ is a nuclear space (the space S say), and if the

[16] P. R. Halmos, *Measure Theory* (D. van Nostrand, Inc., New York, 1950), p. 54.

[17] A. Kolmogorov, *Grundbegriffe der Wahrscheinlichkeitsrechnung, Ergebnisse der Mathematik* (Springer-Verlag, Berlin, 1933), Vol. 2, No. 3; I. M. Gel'fand and N. Y. Vilenkin, *Generalized Functions* (Academic Press Inc., New York, 1964), Vol. 4.

[18] The function $\varphi(F)$ is not to be confused with the "smeared" field operator $\Phi(f)$.

representation $U(f)$ is continuous in this topology, one can confine oneself to the space of continuous functionals.[19]

4. A GENERAL CRITERION FOR KERNEL INTEGRAL FORMULAS

Let $h_1, h_2, \cdots$ be an orthonormal system for $\mathfrak{U}$, and let W_N be the subspace generated by the N first vectors:

$$W_N = \{h_1, \cdots, h_N\}. \tag{4.1}$$

Every $f, g \in W_N$ can be written in the form

$$f = \sum_1^N \alpha_i h_i, \quad g = \sum_1^N \beta_i h_i,$$

and

$$d^N f\, d^N g \equiv d\alpha_1 \cdots d\alpha_N\, d\beta_1 \cdots d\beta_N$$

is the usual Lebesgue measure in $W_N \times W_N$ determined by the scalar product in W_N.

Now we consider

$$I_N(\varphi, \varphi_0, \psi) \equiv \int_{W_n \times W_n} d^N f\, d^N g/(2\pi)^N \langle \varphi, U(f, g)\varphi_0\rangle\langle U(f, g)\varphi_0, \psi\rangle, \tag{4.2}$$

where $\|\varphi_0\| = 1$. The representation $U(f, g)$, if restricted to $f, g \in W_N$, becomes a representation for N degrees of freedom. Thus Eq. (2.31) of Lemma 2.1 applies, and one has the absolute integrability of the integrand in (4.2) as a consequence by Schwarz's inequality. According to Fubini's theorem, the double integral can be replaced by iterated integrals. We are going to see under what condition the integral approaches $\langle \varphi, \psi\rangle$ for $N \to \infty$ or for a subsequence $N_1, N_2, \cdots$.

We assume that φ_0 is cyclic for $U(f)$. The general case will be treated later. In the realization of the representation given by Eq. (3.7), let φ and ψ correspond to $\varphi(F)$ and $\psi(F)$, while $\varphi_0(F) \equiv 1$. One then has

$$\langle \varphi, U(f)V(g)\varphi_0\rangle = \int_{\mathfrak{U}'} d\mu(F)\bar{\varphi}(F)e^{i(F,f)}a_g(F)$$

and a similar expression for the second scalar product. Equation (4.2) becomes

$$I_N = \int_{W_N \times W_N} d^N f\, d^N g/(2\pi)^N \int_{\mathfrak{U}'} d\mu(F)\bar{\varphi}(F)e^{i(F,f)}a_g(F) \times \int_{\mathfrak{U}'} d\mu(F')\bar{a}_g(F')e^{-i(F',f)}\psi(F'). \tag{4.3}$$

The guiding principle for the further investigations in this section comes from the following observation. The integral over $d^N f$ reminds one strongly of a δ function or Fourier transform. However, $\mathfrak{U}'$ is an infinite-dimensional space with the measure μ not further specified. Therefore, one will have to try to reduce the integral over $\mathfrak{U}'$ somehow to a finite-dimensional Lebesgue integral. Of course, this will not be possible without more ado, and we therefore introduce some new notations and a few lemmas. Let

$$\mathfrak{K}_N \equiv \overline{\{U(f)\varphi_0; f \in W_N\}} \triangleq \overline{\{e^{i(F,f)}; f \in W_N\}} \tag{4.4}$$

be the closed subspace of $\mathfrak{K}$ generated by the vectors $U(f)\varphi_0$, $f \in W_N$. In the realization $\mathfrak{K} = L^2_\mu$, $\mathfrak{K}_N$ is generated by the functions $e^{i(F,f)}$, $f \in W_N$. Let P_N be the projection operator onto $\mathfrak{K}_N$. Denote by $\mathfrak{U}_0$ the set of all finite linear combinations of the h_i:

$$\mathfrak{U}_0 \equiv \{h_1, h_2, \cdots\} = \bigcup_N W_N. \tag{4.5}$$

If $\mathfrak{U}$ is finite dimensional, one has of course $\mathfrak{U}_0 = \mathfrak{U}$, and φ_0 is also cyclic for $U(\mathfrak{U}_0)$, i.e., for $U(f)$ with $f \in \mathfrak{U}_0$. If in the infinite case $\mathfrak{U}$ has a suitable topology with respect to which $\mathfrak{U}_0$ is dense in $\mathfrak{U}$, and if $U(f)$ is continuous in this topology, then clearly φ_0 is also cyclic for $U(\mathfrak{U}_0)$. It seems doubtful, however, that one can prove this for the general case. Therefore, whenever needed, we will have to make the additional assumption that φ_0 is also cyclic for $U(\mathfrak{U}_0)$. Later the following simple properties will be needed.

Lemma 4.1: If φ_0 is cyclic for $U(\mathfrak{U}_0)$, then P_N converges strongly to **1** for $N \to \infty$.

Proof: For given $\psi \in \mathfrak{K}$ one has to show that $\lim \|\psi - P_N\psi\| = 0$. For any $\epsilon > 0$ there are numbers $\lambda_1, \cdots, \lambda_n$ and elements $f_1, \cdots, f_n$ of $\mathfrak{U}_0$ such that

$$\|\psi - \sum \lambda_i U(f_i)\varphi_0\| < \epsilon/2.$$

Every f_i lies in a W_{N_i}. Let $N_0 = \max N_i$. Then one has for $N \geq N_0$

$$\|\psi - P_N\psi\| \leq \|\psi - \sum \lambda_i U(f_i)\varphi_0\| + \|\sum \lambda_i U(f_i)\varphi_0 - P_N\psi\| < \epsilon.$$

Lemma 4.2: Let W be a finite-dimensional subspace of $\mathfrak{U}$, and let $\tilde{\mu}$ be the measure in $\mathfrak{U}/W^0$ induced by μ according to lemma 3.1. Let $Z(F)$ be a measurable function on $\mathfrak{U}'$ which is constant within each coset $\tilde{F} \equiv F + W^0$. Then one can consider $Z(\tilde{F})$ as a measurable function[20] on $\mathfrak{U}'/W^0$, and one has

$$\int_{\mathfrak{U}'} d\mu(F)Z(F) = \int_{\mathfrak{U}'/W^0} d\tilde{\mu}(\tilde{F})Z(\tilde{F}). \tag{4.6}$$

[19] I. M. Gel'fand and N. Y. Vilenkin, Ref. 17, last chapter.

[20] One really should introduce another notation for this function, $\tilde{Z}(\tilde{F})$ say, $\tilde{Z}(\tilde{F}) \equiv Z(F)$ for $F \in \tilde{F}$.

Proof: The statement immediately follows from the definition of $\tilde{\mu}$ in (3.6) and from the properties of the integral.

Lemma 4.3: $\mathcal{H}_N$ consists just of those functions of L^2_μ which are constant within each coset $F + W_N^0$ of $\mathfrak{V}'/W_N^0$.

Proof: Let $F_0 \in W_N^0$. Then

$$e^{i(F+F^0,f)} = e^{i(F,f)}$$

for all $f \in W_N$ since $(F_0, f) = 0$. Hence for $f \in W_N$, $\exp[i(F,f)]$ is constant within a coset $F + W_N^0$, and the same holds for finite linear combinations and limits of these. Conversely, let $Z(F) \in L^2_\mu$ be a function with $Z(F + W_N^0) = Z(F)$. Putting $\tilde{F} \equiv F + W_N^0$, one can consider $Z(\tilde{F})$ as a function on $\mathfrak{V}'/W_N^0$ which is square integrable with respect to the measure $\tilde{\mu}_N$ induced in $\mathfrak{V}'/W_N^0$ by μ. Therefore $Z(\tilde{F})$ can be approximated in $L^2_{\tilde{\mu}_N}$ by linear combinations of $\exp[i(\tilde{F}, f)]$, $f \in W_N$, because these functions are dense in $L^2_{\tilde{\mu}_N}$ [according to Eq. (3.5), every $\tilde{F} \in \mathfrak{V}'/W_N^0$ can be considered as a linear functional on W_N]:

$$\int \left| Z(\tilde{F}) - \sum_1^n \lambda_i e^{i(\tilde{F}, f_i)} \right|^2 d\tilde{\mu}_N(\tilde{F}) < \epsilon, \quad f_i \in W_N. \tag{4.7}$$

By lemma 4.2 this shows that $Z(F)$ can be approximated by linear combinations of functions of $\mathcal{H}_N$ and hence lies itself in $\mathcal{H}_N$. Q.E.D.

Now we return to the evaluation of I_N in (4.3) and first take[21] for φ, ψ elements of $\mathcal{H}_M$, $M \leq N$ and M fixed. As a reminder, we write φ_M, ψ_M. We decompose $a_g(F)$ into its two orthogonal components $a_g(F)_N$ and $a_g(F)_{N\perp}$ in $\mathcal{H}_N$ and $\mathcal{H}_{N\perp} \equiv (1 - P_N)\mathcal{H}$, respectively:

$$a_g(F) = a_g(F)_N + a_g(F)_{N\perp}. \tag{4.8}$$

Note that $a_g(F) \in L^2_\mu$ since $a_g(F) = (V(g)\varphi_0)(F)$. According to the last lemma and because of $M \leq N$, one has

$$\begin{aligned} e^{-i(F,f)}\varphi_M(F) &\in \mathcal{H}_N, \\ e^{-i(F,f)}\psi_M(F) &\in \mathcal{H}_N. \end{aligned} \tag{4.9}$$

Inserting (4.8) into (4.3), (4.9) and by the orthogonality of $\mathcal{H}_N$ and $\mathcal{H}_{N\perp}$ one obtains

$$\begin{aligned} I_N = &\int_{W_N \times W_N} d^N f\, d^N g/(2\pi)^N \\ &\times \int_{\mathfrak{V}'} d\mu(F) e^{i(\tilde{F},f)} \bar{\varphi}_M(F) a_g(F)_N \\ &\times \int_{\mathfrak{V}'} d\mu(F') a_g(F')_N e^{-i(\tilde{F}',f)} \psi_M(F'). \end{aligned} \tag{4.10}$$

[21] This is a decisive point of this paper.

The integrands depending on F and F' are now constant within each coset $\tilde{F} \equiv F + W_N^0$. By lemma 4.2 one, therefore, gets

$$\begin{aligned} I_N = &\int_{W_N \times W_N} d^N f\, d^N g/(2\pi)^N \\ &\times \int_{\mathfrak{V}'/W_N{}^0} d\tilde{\mu}_N(\tilde{F}) e^{i(\tilde{F},f)} \bar{\varphi}_M(\tilde{F}) a_g(\tilde{F})_N \\ &\times \int_{\mathfrak{V}'/W_N{}^0} d\tilde{\mu}_N(\tilde{F}') \bar{a}_g(\tilde{F}')_N e^{-i(\tilde{F}',f)} \psi_M(\tilde{F}'), \end{aligned} \tag{4.11}$$

where $\tilde{\mu}_N$ is the measure in $\mathfrak{V}'/W_N^0$ induced by μ.

Lemma 4.4: The measure $\tilde{\mu}_N$ is quasi-invariant.

Proof: One has to show that $\tilde{\mu}_N(A) = 0$ implies $\tilde{\mu}_N(A + \tilde{g}) = 0$ for every $\tilde{g} \in \mathfrak{V}'/W_N^0$, where A is a nonempty subset of $\mathfrak{V}'/W_N^0$. Let $Z \subset \mathfrak{V}'$ be the cylinder set belonging to base A and generating subspace W_N. By (3.6) one has $\mu(Z) = \tilde{\mu}_N(A) = 0$. According to Eqs. (3.4) and (3.5), there lies an element $g \in W_N$ in each coset $\tilde{g} \in \mathfrak{V}'/W_N^0$. Choose this g as a representative for $\tilde{g}$, $\tilde{g} = g + W_N^0$. If η is the natural homomorphism of $\mathfrak{V}'$ onto $\mathfrak{V}'/W_N^0$, then

$$\eta^{-1}(A + \tilde{g}) = Z + g + W_N^0 = Z + g.$$

Therefore $Z + g$ is a cylinder set with base $A + \tilde{g}$ and generating subspace W_N. The quasi-invariance of μ implies $\mu(Z + g) = 0$, and therefore

$$\tilde{\mu}_N(A + \tilde{g}) = \mu(Z + g) = 0. \quad \text{Q.E.D.}$$

Every normed quasi-invariant measure on the Borel sets of a real N-dimensional vector space ($N < \infty$) is equivalent to the Lebesgue measure.[22] Hence there exists a positive measurable function[23] $\rho_N(F)$ on $\mathfrak{V}'/W_N^0$ such that

$$d\tilde{\mu}_N(\tilde{F}) = \rho_N(\tilde{F})\, d^N\tilde{F}, \tag{4.12}$$

where $d^n\tilde{F}$ is given by the Lebesgue measure in $\mathfrak{V}'/W_N^0$ which is induced by the Lebesgue measure in W_N through the identification of W_N and $\mathfrak{V}'/W_N^0$ in Eq. (3.5).[24] Since μ and $\tilde{\mu}_N$ are normed, one has

$$\int_{\mathfrak{V}'/W_N{}^0} \rho_N(\tilde{F})\, d^N\tilde{F} = 1. \tag{4.13}$$

[22] I. M. Gel'fand and N. Y. Vilenkin, Ref. 17, p. 352, Theorem 2.
[23] I. M. Gel'fand and N. Y. Vilenkin, Ref. 17, p. 351, Theorem 1.
[24] For $f \in W_N$ and $g = 0$, the vacuum functional is related to $\rho_N(\tilde{F})$ by a Fourier transformation. By Eq. (3.7) one has

$$E(f, 0) = \int \exp\{i(\tilde{F}, f)\} \rho_N(\tilde{F})\, d^N\tilde{F}$$

for $f \in W_N$.

Equation (4.11) now becomes

$$I_N = \int_{W_N \times W_N} d^N f\, d^N g/(2\pi)^N \times \int_{\mathfrak{V}'/W_N^0} d^N \tilde{F} e^{i(\tilde{F},f)} \rho_N(\tilde{F}) \bar{\varphi}_M(\tilde{F}) a_g(\tilde{F})_N \times \int_{\mathfrak{V}'/W_N^0} d^N \tilde{F}' e^{-i(\tilde{F}',f)} \rho_N(\tilde{F}') \bar{a}_g(\tilde{F}')_N \psi_M(\tilde{F}'). \tag{4.14}$$

Formal integration over $d^N f/(2\pi)^N$ gives $\delta^{(N)}(\tilde{F} - \tilde{F}')$, and subsequent integration over $d^N\tilde{F}'$ leads to

$$I_N(\varphi_M, \varphi_0, \psi_M) = \int_{W_N} d^N g \int_{\mathfrak{V}'/W_N^0} d^N \tilde{F} \rho_N^2(\tilde{F}) |a_g(\tilde{F})_N|^2 \bar{\varphi}_M(\tilde{F}) \psi_M(\tilde{F}). \tag{4.15}$$

We now justify Eq. (4.15) in a rigorous manner.

Lemma 4.5: Let $\varphi_M, \psi_M \in \mathcal{H}_M$ with $M \leq N$. Then $I_N(\varphi_M, \varphi_0, \psi_M)$ is given by Eq. (4.15).

Proof: First let φ_M, ψ_M be such that

$$|\varphi_M(\tilde{F})| \{\rho_N(\tilde{F})\}^{\frac{1}{2}}$$

and $|\psi_M(\tilde{F})| \{\rho_N(\tilde{F})\}^{\frac{1}{2}}$ are bounded:

$$|\varphi_M(\tilde{F})| \{\rho_N(\tilde{F})\}^{\frac{1}{2}} \leq C_\varphi < \infty, \quad |\psi_M(\tilde{F})| \{\rho_N(\tilde{F})\}^{\frac{1}{2}} \leq C_\psi < \infty. \tag{4.16}$$

The set of these vectors for $M = 1, \cdots, N$ is dense in $\mathcal{H}_N$ since, according to (4.12), the mapping

$$\varphi(\tilde{F}) \leftrightarrow \varphi'(\tilde{F}) \equiv \varphi(\tilde{F}) \{\rho_N(\tilde{F})\}^{\frac{1}{2}} \tag{4.17}$$

of $L^2_{\tilde{\mu}_N}(\tilde{F})$ onto $L^2(\tilde{F})$ is isometric and since the bounded functions are dense in $L^2(\tilde{F})$, where $L^2(\tilde{F})$ denotes the space of all Lebesgue-square-integrable (L^2) functions on $\mathfrak{V}'/W_N^0$. From $a_g(\tilde{F})_N \in L^2_{\tilde{\mu}_N}(\tilde{F})$ it follows that $a_g(\tilde{F})_N \{\rho_N(\tilde{F})\}^{\frac{1}{2}} \in L^2(\tilde{F})$. Therefore, the integrands of the two integrals over $d^N\tilde{F}$ and $d^N\tilde{F}'$ in Eq. (4.14) are L^2 functions so that Parseval's formula for Fourier transforms of L^2 functions can be applied to the integral over $d^N f/(2\pi)^N$. This immediately gives Eq. (4.15) for functions of the form of Eq. (4.16).

In order to prove (4.15) for arbitrary elements of $\mathcal{H}_M$, we use the linearity of $I(\varphi, \varphi_0, \psi)$ in φ and ψ. Since one can decompose every function in real and imaginary part and these in positive and negative part, it suffices to prove (4.15) for nonnegative $\varphi_M(F)$ and $\psi_M(F)$.

Define $\varphi'_M(\tilde{F})$ and $\psi'_M(\tilde{F})$ as $\varphi'(\tilde{F})$ in Eq. (4.17). Since $\varphi'_M, \psi'_M \in L^2(\tilde{F})$, it follows[25] that there exists an increasing sequence of nonnegative bounded L^2 functions $\varphi'_\nu(\tilde{F})$, such that

$$\lim_\nu \varphi'_\nu(\tilde{F}) = \varphi'_M(\tilde{F}) \tag{4.18}$$

almost everywhere and

$$\lim_\nu \int d^N \tilde{F} |\varphi'_M(\tilde{F}) - \varphi'_\nu(\tilde{F})|^2 = 0. \tag{4.19}$$

An analogous sequence ψ'_ν exists for $\psi'_M(F)$. Then φ_ν, ψ_ν,

$$\varphi_\nu(\tilde{F}) \equiv \varphi'_\nu(\tilde{F}) \{\rho_N(\tilde{F})\}^{-\frac{1}{2}}, \quad \psi_\nu(\tilde{F}) \equiv \psi'_\nu(\tilde{F}) \{\rho_N(\tilde{F})\}^{-\frac{1}{2}}, \tag{4.20}$$

are elements of $L^2_{\tilde{\mu}_N} \triangleq \mathcal{H}_N$, for which Eq. (4.19) reads

$$\lim_\nu \|\varphi_M - \varphi_\nu\|^2 = 0, \quad \lim_\nu \|\psi_M - \psi_\nu\|^2 = 0.$$

Equation (2.31) and the continuity properties of $I_N(\varphi_\nu, \varphi_0, \psi_{\nu'})$ resulting therefrom imply

$$\lim_\nu \left(\lim_{\nu'} I_N(\varphi_\nu, \varphi_0, \psi_{\nu'}) \right) = I_N(\varphi_M, \varphi_0, \psi_M). \tag{4.21}$$

But φ_ν and ψ_ν satisfy Eq. (4.15). Since the sequences are increasing and since the functions are nonnegative, one obtains[26] for the left-hand side of Eq. (4.21)

$$\lim_\nu \left(\lim_{\nu'} \int d^N g \int d^N \tilde{F} \varphi_\nu(\tilde{F}) \psi_{\nu'}(\tilde{F}) |a_g(\tilde{F})_N|^2 \rho_N^2(\tilde{F}) \right) = \int d^N g \int d^N \tilde{F} \varphi_M \psi_M |a_g(\tilde{F})_N|^2 \rho_N^2. \quad \text{Q.E.D.}$$

Before formulating the promised criterion, we prove the following lemma:

Lemma 4.6: For all $\varphi_M, \psi_M \in \mathcal{H}_M$, $M \leq N$, one has

$$\int_{W_N} d^N g \int_{\mathfrak{V}'} d\mu(F) |a_g(F)|^2 \rho_N(F) \bar{\varphi}_M(F) \psi_M(F) = \langle \varphi_M, \psi_M \rangle, \tag{4.22}$$

where $\rho_N(F)$ is defined[27] by $\rho_N(F) \equiv \rho_N(\tilde{F})$ for $F \in \tilde{F}$.

Proof: By (3.9) one has $d\mu(F) \cdot |a_g(F)|^2 = d\mu(F + g)$. Changing the variable F into $F - g$, one obtains for the left-hand side of Eq. (4.22)

$$\int_{W_N} d^N g \int_{\mathfrak{V}'} d\mu(F) \rho_N(F - g) \bar{\varphi}_M(F - g) \psi_M(F - g).$$

[25] P. R. Halmos, Ref. 15, Theorem B on p. 85 and Theorem D on p. 110.

[26] P. R. Halmos, Ref. 25, Theorem B on p. 112.

[27] Cf. the notational remark in footnote 20.

The integrand is constant within each coset of $\mathfrak{U}'/W_N^0$. Thus, by lemma 4.2 and Eq. (4.12), this expression becomes

$$\int_{W_N} d^N g \int_{\mathfrak{U}'/W_N^0} d^N\tilde{F}\rho_N(\tilde{F})\rho_N(\tilde{F}-\tilde{g}) \times \bar{\varphi}_M(\tilde{F}-\tilde{g})\psi_M(\tilde{F}-\tilde{g}),$$

where $\tilde{g} = g + W_N^0$. However, for $g \in W_N$ the mapping $g \to \tilde{g}$ is an isomorphism, by Eq. (3.5); and, according to the particular choice of the Lebesgue measure, $d^N\tilde{g} = d^N g$ holds. We can thus write $\tilde{F} - \tilde{g} = \tilde{F} - g$ in the integrand, and another change of the variable yields

$$\int_{W_N} d^N g \int_{\mathfrak{U}'} d\mu(F)\,|a_g(F)|^2\,\rho_N(F)\bar{\varphi}_M(F)\psi_M(F) = \int_{W_N} d^N g \int_{\mathfrak{U}'/W_N^0} d\tilde{\mu}_N(\tilde{F})\rho_N(\tilde{F}+g)\bar{\varphi}_M(\tilde{F})\psi_M(\tilde{F}). \tag{4.23}$$

Decomposing $\varphi_M(\tilde{F})$, $\psi_M(\tilde{F})$ into real and imaginary part and then into negative and nonnegative part, one can assume $\varphi_M(\tilde{F})$ and $\psi_M(\tilde{F})$ to be nonnegative. Then the order of integration can be interchanged. By Eq. (4.13) the integral over $d^N g$ is 1. Applying lemma 4.2 to the remaining integral just yields $\langle \varphi_M, \psi_M \rangle$. Q.E.D.

Now we are in a position to prove the criterion.

Theorem 4.1: Let $n_1 < n_2 < \cdots$ be a sequence of natural numbers. Let $h_1, h_2, \cdots$ be a basis of $\mathfrak{U}$ and denote by $\mathfrak{U}_0 = \{h_1, h_2, \cdots\}$ the set of all finite linear combinations of the h_i and, correspondingly, $W_n = \{h_1, \cdots, h_n\}$. Let $U(f, g)$ with $f, g \in \mathfrak{U}$ be a representation of the CCR in which $U(\mathfrak{U}_0)$ is cyclic, with cyclic vector φ_0 say, $\|\varphi_0\| = 1$. *Then*

$$\lim_{i\to\infty} \int_{W_{n_i}\times W_{n_i}} d^{n_i}f\, d^{n_i}g/(2\pi)^{n_i} \times \langle \varphi, U(f, g)\varphi_0\rangle\langle U(f, g)\varphi_0, \psi\rangle = \langle \varphi, \psi\rangle \tag{4.24}$$

for all $\varphi, \psi \in \mathfrak{K}$ *if and only if* for any $\varphi_M, \psi_M \in \mathfrak{K}_M$, $M = 1, \cdots, M < \infty$,

$$\lim_{i\to\infty} \int_{W_{n_i}} d^{n_i}g \int_{\mathfrak{U}'} d\mu(F) \times \rho_{n_i}(F)\{|a_g(F)|^2 - |a_g(F)_{n_i}|^2\}\bar{\varphi}_M\psi_M = 0. \tag{4.25}$$

Proof: Since one can assume $n_i \geq M$, the necessity of Eq. (4.25) follows immediately from lemmas 4.5 and 4.6 if one puts $\varphi = \varphi_M$ and $\psi = \psi_M$. Now assume Eq. (4.25) to hold. Then (4.24) holds for $\varphi = \varphi_M$, $\psi = \psi_M$, by the same argument. Now let φ and ψ be arbitrary vectors in $\mathfrak{K}$. In view of the linearity of I_n, one can take φ and ψ to be unit vectors. Let $\epsilon > 0$, $1 \geq \epsilon$ and arbitrary otherwise. Put $\epsilon' = \epsilon/5$. Since φ_0 is cyclic for $U(\mathfrak{U}_0)$, there is an M, $M < \infty$, and vectors $\varphi_M, \psi_M \in \mathfrak{K}_M$ such that $\|\varphi_M\|, \|\psi_M\| \leq 1$ and $\|\varphi - \varphi_M\| < \epsilon'$, $\|\psi - \psi_M\| < \epsilon'$. Using the linearity of I_n, by the second part of lemma 2.1 one obtains

$$\begin{aligned}|I_n(\varphi, \varphi_0, \psi) - I_n(\varphi_M, \varphi_0, \psi_M)| &= |I_n((\varphi - \varphi_M) + \varphi_M, \varphi_0, (\psi - \psi_M) + \psi_M) \\ &\quad - I_n(\varphi_M, \varphi_0, \psi_M)| \leq \epsilon' + \epsilon' + \epsilon'. \end{aligned}\tag{4.26}$$

Hence

$$\begin{aligned}\overline{\lim_{i\to\infty}} |I_{n_i}(\varphi, \varphi_0, \psi) - \langle \varphi, \psi\rangle| &\leq \overline{\lim_{i\to\infty}} |I_{n_i}(\varphi, \varphi_0, \psi) - I_{n_i}(\varphi_M, \varphi_0, \psi_M)| \\ &\quad + \overline{\lim_{i\to\infty}} |I_{n_i}(\varphi_M, \varphi_0, \psi_M) - \langle \varphi, \psi\rangle| \\ &\leq 3\epsilon' + |\langle \varphi_M, \psi_M\rangle - \langle \varphi, \psi\rangle| \\ &\leq 3\epsilon' + 2\epsilon' = \epsilon. \end{aligned}\tag{4.27}$$

Thus the limit superior of the left-hand side is zero. Since all numbers are positive, this implies that the limit exists and is equal to zero. Q.E.D.

The condition in Eq. (4.25) of Theorem 4.1 means that $a_g(F)_n$ has to tend in a particular way towards $a_g(F)$ in order for the kernel integral to assume the correct value. Recall that $a_g(F)_n$ is the projection $P_n(V(g)\varphi_0)$ of $V(g)\varphi_0$ onto $\mathfrak{K}_n$. Since by lemma 4.1 P_n converges strongly to **1**, $a_g(F)_n$ converges to $a_g(F)$ in norm. The only question is whether or not this convergence is so rapid that the integral in Eq. (4.25) goes to zero. We return to this question in Sec. 7.

5. APPLICATION TO PARTIAL TENSOR-PRODUCT REPRESENTATIONS AND OTHER SPECIAL CASES

The preceding theorem holds independently of the dimension of $\mathfrak{U}$. For finitely many degrees of freedom, $\mathfrak{U}$ is finite dimensional, dim $\mathfrak{U} = N$ say, and one has $\mathfrak{U} = \mathfrak{U}_0 = \mathfrak{U}'$ and

$$\mathfrak{K}_N = \overline{\{U(W_N)\varphi_0\}} = \overline{\{U(V)\varphi_0\}} = \mathfrak{K}$$

if φ_0 is cyclic for $U(V)$. Therefore

$$a_g(F)_N = a_g(F) \tag{5.1}$$

for all $g \in \mathfrak{U}$. This Eq. (4.25) is trivially fulfilled, and one obtains Eq. (2.29) for all cyclic φ_0. Since in the Schrödinger representation $U(\mathfrak{U})$ is cyclic, and since the set of cyclic vectors is dense on the unit sphere,

Eq. (2.29) follows for all unit vectors φ_0 by continuity reasons. In this way one has reproduced the kernel integral for the Schrödinger representation. We point out, however, that in the proof of Theorem 4.1 use has been made of square integrability of $\varphi(f, g)$, so that for a complete proof for the finite case this has to be shown without Eq. (2.31). This is not difficult.

If $\mathfrak{U}$ is infinite dimensional, Eq. (5.1) is not true in general. There are, however, classes of representations in which Eq. (3.1) is true either for all N or at least for a sequence $n_1 < n_2 < \cdots$. It will be shown in Paper II that these are just the partial tensor-product representations. Here we briefly discuss these representations. For direct- or tensor-product representations a kernel integral formula is known[5,11]; in our discussion this formula results from a simple specialization of partial tensor-product representations and Theorem 4.1. In order to define these representations we have to make a few remarks on incomplete tensor products of Hilbert spaces introduced by von Neumann.[28]

Let J be an index set. Let z_α, $\alpha \in J$, be complex numbers. Then

$$\prod_{\alpha \in J} z_\alpha \tag{5.2}$$

is called convergent[28] with value a if for any $\delta > 0$ there exists a finite subset $J_0(\delta)$ such that, for each finite set $J' = (\alpha_1, \cdots, \alpha_n)$ with $J_0 \subset J' \subset J$,

$$|z_{\alpha_1} \cdots z_{\alpha_n} - a| \leq \delta. \tag{5.3}$$

The product in (5.2) is called quasiconvergent if the product of the absolute values of the z_α is convergent. If it even converges in the above sense, its value is a; if it does not converge, the value 0 is assigned to it.

Now let $\mathfrak{H}_\alpha$, $\alpha \in J$, be a set of Hilbert spaces. A sequence of vectors φ_α, $\varphi_\alpha \in \mathfrak{H}_\alpha$, is called a C sequence if the product of the $\|\varphi_\alpha\|$ converges. If ψ_α is another C sequence, then $\prod_{\alpha \in J} \langle \varphi_\alpha, \psi_\alpha \rangle$ is quasiconvergent.[28]

The *complete direct or tensor product* $\bigotimes_{\alpha \in J} \mathfrak{H}_\alpha$ now consists of the closure of the linear hull of the "product vectors" $\bigotimes \varphi_\alpha$, where φ_α belongs to a C sequence. The scalar product is defined in the sense of quasiconvergence by

$$\langle \bigotimes \varphi_\alpha, \bigotimes \psi_\alpha \rangle \equiv \prod_{\alpha \in J} \langle \varphi_\alpha, \psi_\alpha \rangle.$$

Here a product vector $\bigotimes \varphi_\alpha$ is nothing but a function on J which associates every $\alpha \in J$ with a vector $\varphi_\alpha \in \mathfrak{H}_\alpha$. Thereby the complete direct product is independent of any ordering of J, i.e., it is commutative.

Let a sequence of unit vectors $\varphi_\alpha^0 \in \mathfrak{H}_\alpha$ be given. The *incomplete direct* or *tensor product* (ITP)

$$\mathfrak{H}\varphi^0 \equiv \bigotimes_{\alpha \in J}^{(\otimes \varphi_\alpha^0)} \mathfrak{H}_\alpha \tag{5.4}$$

of the $\mathfrak{H}_\alpha$ with respect to the reference vector $\varphi^0 = \bigotimes \varphi_\alpha$ is now defined as the closed linear subspace of the complete tensor product which is generated by all vectors of the form

$$\varphi = \bigotimes \varphi_\alpha \quad \text{with} \quad \varphi_\alpha = \varphi_\alpha^0 \text{ except for finitely many } \alpha. \tag{5.5}$$

By definition the ITP is commutative.

Two product vectors $\bigotimes \varphi_\alpha$, $\bigotimes \psi_\alpha$ with $0 < \prod \|\varphi_\alpha\| < \infty$ and $0 < \prod \|\psi_\alpha\| < \infty$ are called equivalent if

$$\sum_{\alpha \in J} |\langle \varphi_\alpha, \psi_\alpha \rangle - 1| < \infty, \tag{5.6}$$

where only countably many nonvanishing terms are allowed in the sum. One can show the following[28]: If $\bigotimes \varphi_\alpha^0$ is reference vector of an ITP, and if $\bigotimes \psi_\alpha$ is equivalent to $\bigotimes \varphi_\alpha^0$, then $\bigotimes \psi_\alpha$ lies in the ITP determined by $\bigotimes \varphi_\alpha^0$. Thus equivalent reference vectors define the same ITP. Different ITP are pairwise orthogonal.[28]

Partial tensor products are a simple generalization of ITP. Decompose the index set J into finite subsets J_r:

$$J = \bigcup_r J_r.$$

For every r form the usual finite tensor product

$$\mathfrak{K}(r) = \bigotimes_{\alpha \in J_r} \mathfrak{H}_\alpha; \tag{5.7}$$

choose some unit vector ψ_r^0 from each $\mathfrak{K}(r)$, and form the ITP of the $\mathfrak{K}(r)$ with respect to ψ_r^0:

$$\mathfrak{K} = \bigotimes_r^{(\otimes \psi_r^0)} \mathfrak{K}(r). \tag{5.8}$$

The resulting Hilbert space $\mathfrak{K}$ is called a *partial tensor product* (PTP). It differs from an ITP in the reference vector because it need not be a product vector with respect to the original $\mathfrak{H}_\alpha$.

Now the corresponding representations of the CCR will be defined. Let $h_1, h_2, \cdots$ be a basis of the test function space $\mathfrak{U}$, and let every element of $\mathfrak{U}$ be a finite linear combination of the h_i, i.e., $\mathfrak{U} = \mathfrak{U}_0$. Let J be the set of natural numbers. Let all $\mathfrak{H}_\alpha$ be isomorphic to $L^2(R^1)$, the space of square-integrable functions of one variable; let in each $\mathfrak{H}_\alpha$ a Schrödinger representation of $[Q, P] = i$ be given, and denote the corresponding Weyl operators by $\tilde{U}_\alpha(p)$, $\tilde{V}_\alpha(q)$ [cf. Eq. (2.27)]. One defines unitary operators $U_n(p)$, $V_n(p)$ in $\bigotimes \mathfrak{H}_\alpha$ by

$$U_n(p) = \tilde{U}_n(p) \otimes \left(\bigotimes_{\alpha \neq n} \mathbf{1}_\alpha \right),$$

$$V_n(q) = \tilde{V}_n(q) \otimes \left(\bigotimes_{\alpha \neq n} \mathbf{1}_\alpha \right). \tag{5.9}$$

[28] J. von Neumann, Comp. Math. **6**, 1 (1938).

Now let $f, g \in \mathfrak{U}$,

$$f = \sum_1^N p_n h_n, \quad g = \sum_1^M q_n h_n.$$

We define

$$U(f) \equiv \prod_1^N U_n(p_n), \quad V(g) \equiv \prod_1^M V_n(q_n). \quad (5.10)$$

This is obviously a representation of the CCR. However, it is reducible in $\otimes \mathcal{H}_\alpha$. For let $\mathcal{H}_{\varphi 0}$ be the ITP defined by Eqs. (5.4) and (5.5). Every $U(f)$, $V(g)$ changes only a finite number of factors in a product vector, so that by Eq. (5.5) $\mathcal{H}_{\varphi 0}$ is invariant. The irreducibility of the Schrödinger representation implies that $\mathcal{H}_{\varphi 0}$ is irreducible under $U(f, g)$.[29] If every φ_α^0 is cyclic for $\tilde{U}_\alpha(p)$, then obviously $\otimes \varphi_\alpha^0$ is cyclic for $U(f)$. The representation defined by Eq. (5.10) in an ITP $\mathcal{H}_{\varphi 0}$ is called a *direct* or *tensor-product representation* (TPR) with respect to the basis h_i of $\mathfrak{U}$.

In the same way one can define a *partial tensor-product representation* (PTPR) with respect to a basis h_i of $\mathfrak{U}$. Decompose the set J of natural numbers into finite subset J_r, $r = 1, 2, \cdots$, and form a PTP $\mathcal{H}_{\varphi 0}$, as in Eq. (5.8). Let $\nu(r)$ be the number of elements of J_r. In each $\mathcal{H}(r)$ define a Schrödinger representation for $\nu(r)$ degrees of freedom analogously to Eq. (5.9): i.e., if $n \in J_r$, take

$$\hat{U}_n(p) = \tilde{U}_n(p) \otimes \left(\bigotimes_{\substack{\alpha \in Jr \\ \alpha \neq n}} \mathbf{1}_\alpha \right) \quad (5.11)$$

as operators in $\mathcal{H}(r)$; similarly for $\hat{V}_n(q)$. In $\otimes \mathcal{H}(r)$ one defines operators $U_n(p)$,

$$U_n(p) = \hat{U}_n(p) \otimes \left(\bigotimes_{r' \neq r} \mathbf{1}_{r'} \right), \quad (5.12)$$

and similarly $V_n(q)$. Then $U(f)$ and $V(g)$ are defined as in Eq. (5.10). Again $U(f, g)$ is irreducible in $\mathcal{H}_{\varphi 0}$. By a renumbering of the basis vectors h_i and of the index set J, one can transform the subsets J_r into intervals:

$$J_1 = (1, \cdots, n_1), \quad J_2 = (n_1 + 1, \cdots, n_2), \cdots. \quad (5.13)$$

In the following we will always assume this kind of ordering.

If each ψ_r^0 in the reference vector $\otimes \psi_r^0$ is cyclic for

$$\hat{U}_r(p_1, \cdots, p_{n_r}) \equiv \hat{U}_{n_{r-1}+1}(p_1) \cdots \hat{U}_{n_r}(p_{n_r}),$$

then obviously $\otimes \psi_r^0$ is cyclic for $U(f)$. We now show that one can always assume $\otimes \psi_r^0$ to be cyclic.

Lemma 5.1: Let $U(f, g)$ be a TPR or PTPR in $\mathcal{H}_{\varphi 0} = \otimes^{(\otimes \psi_r 0)} \mathcal{H}(r)$. Then in each $\mathcal{H}(r)$ there exists a unit vector $\tilde{\psi}_r^0$ such that $\mathcal{H}_{\psi 0} = \mathcal{H}_{\tilde{\varphi} 0}$ and such that $\tilde{\psi}^0 \equiv \otimes \tilde{\psi}_r^0$ is cyclic for $U(f)$.

Proof: A TPR is a special case of a PTPR, so we treat only the latter. In each $\mathcal{H}(r)$ the vectors cyclic with respect to $\hat{U}_r(p_1, \cdots, p_n)$ are dense on the unit sphere. From these one can choose a $\tilde{\psi}_r^0$ in such a way that $\|\tilde{\psi}_r^0 - \psi_r^0\| < 2^{-r}$. Then

$$|\langle \tilde{\psi}_r^0, \psi_r^0 \rangle - 1| = |\langle \tilde{\psi}_r^0 - \psi_r^0, \psi_r^0 \rangle| < 2^{-r}$$

and

$$\sum_r |\langle \tilde{\psi}_r^0, \psi_r^0 \rangle - 1| < \infty.$$

Thus $\otimes \tilde{\psi}_r^0$ is equivalent to $\otimes \psi_r^0$, hence $\otimes \tilde{\psi}_r^0 \in \mathcal{H}_{\psi 0}$, and thus $\mathcal{H}_{\tilde{\psi} 0} = \mathcal{H}_{\psi 0}$. The reference vector $\otimes \tilde{\psi}_r^0$ is cyclic for $U(f)$. Q.E.D.

Now the application of the criterion of the preceding section is straightforward. Let

$$W_n = \{h_1, \cdots, h_n\} \quad \text{and} \quad \mathcal{H}_n = \overline{\{U(W_n)\psi^0\}},$$

where the reference vector $\psi^0 = \otimes \psi_r^0$ is taken to be cyclic. Then it follows immediately from the definition of a PTPR in Eqs. (5.12), (5.13), and (5.10) that

$$V(W_{n_i})\psi^0 \subset \mathcal{H}_{n_i}, \quad (5.14)$$

hence

$$a_g(F)_{n_i} = a_g(F) \quad \text{for} \quad g \in W_{n_i}, \quad i = 1, 2, \cdots, \quad (5.15)$$

where the n_i are given by Eq. (5.13). For a TPR one has in particular $n_i = i$, since in this case the J_i consist of only one point. Theorem 4.1 thus implies the following corollary:

Corollary 5.1: Let $U(f, g)$ be a PTPR as defined in Eqs. (5.12), (5.13), and (5.10) with respect to the basis $h_1, h_2, \cdots$ of $\mathfrak{U}$. Choose the reference vector $\varphi^0 = \otimes \varphi_r^0$ to be cyclic. Then

$$\lim_{i \to \infty} \int_{W_{n_i} \times W_{n_i}} d^{n_i} f \, d^{n_i} g / (2\pi)^{n_i} \langle \varphi, U(f, g)\varphi_0 \rangle \times \langle U(f, g)\varphi_0, \psi \rangle = \langle \varphi, \psi \rangle \quad (5.16)$$

for all $\varphi, \psi \in \mathfrak{H}$. The n_i are given by Eq. (5.13). In case of a TPT, one has $n_i = i$.

In Paper II it will turn out that one can take any unit vector for φ_0 in Eq. (5.16). For TPR, Eq. (5.16) has been shown by Klauder and McKenna,[11] and a complete classification of TPR up to unitary equivalence has been given in Ref. 5. We note that for TPR the above result obviously holds independently of the ordering of the basis $h_1, h_2, \cdots$ of $\mathfrak{U}$. For PTPR this need not be true.

[29] This follows from Ref. 28, Theorem IX.

6. SHARPENING OF THE CRITERION

In this section the criterion of Theorem 4.1 will be sharpened considerably. It will turn out that Eq. (4.25) need hold only for $\varphi_M(F) = \psi_M(F) = \varphi_0(F) \equiv 1$. This in turn just means that the integrals over $|E(f,g)|^2$ tend to 1, where $E(f,g) = \langle \varphi_0, U(f,g)\varphi_0 \rangle$ is the vacuum functional belonging to φ_0. The criterion is then carried over to the basis-independent kernel integral of Eq. (2.36). Again it turns out to be sufficient to consider only the vacuum functional. The important point for both the limit superior and the supremum over all bases is that one can replace these by a limit over a subsequence which is independent of φ and ψ.

Using the same notation as in Sec. 4, we first prove a theorem for the kernel integral as a limit superior and get, as a consequence of the proof, a corollary for the kernel integral as an ordinary limit.

Theorem 6.1: Let $h_1, h_2, \cdots$ be a basis of $\mathfrak{V}$, and let $U(f,g)$ be a representation of the CCR with cyclic $U(\mathfrak{V}_0)$. Let the unit vector φ_0 be cyclic for $U(\mathfrak{V}_0)$. Then the following statements are equivalent:

(a) $\overline{\lim_n} I_n(\varphi_0, \varphi_0, \varphi_0) = 1$;

(b) $\overline{\lim_n} I_n(\varphi, \varphi_0, \varphi) = \|\varphi\|^2$, for all $\varphi \in \mathcal{H}$;

(c) There exists a subsequence $n_1 < n_2 < \cdots$ such that for all $\varphi, \psi \in \mathcal{H}$,

$$\lim_{i \to \infty} I_{n_i}(\varphi, \varphi_0, \psi) = \langle \varphi, \psi \rangle;$$

(d) There exists a subsequence $n_1 < n_2 < \cdots$ such that

$$\lim_i \int_{W_{n_i}} d^{n_i}g \int_{\mathfrak{V}'} d\mu(F) \times \rho_{n_i}(F)\{|a_g(F)|^2 - |a_g(F)_{n_i}|^2\} = 0.$$

Proof: We show (a) → (d) → (c) → (b) → (a).

(a) → (d): There exists a subsequence $n_1 < n_2 < \cdots$ such that $I_{n_i}(\varphi_0, \varphi_0, \varphi_0)$ converges to the limit superior. By lemmas 4.5 and 4.6, with φ_M and ψ_M replaced by φ_0, this is just (d).

(d) → (c): First we show that condition (4.25) is fulfilled for *bounded* functions. Let $M \leq n$ and let $\varphi_M(F)$, $\psi_M(F)$ be bounded functions lying in $\mathcal{H}_M$. By lemma 4.2 and Eq. (4.23) one has

$$\begin{aligned} K_n &\equiv \int_{W_n} d^n g \int_{\mathfrak{V}'} d\mu(F) \rho_n(F)\{|a_g(F)|^2 \\ &\quad - |a_g(F)_n|^2\} \bar{\varphi}_M(F)\psi_M(F) \\ &= \int_{W_n} d^n g \int_{\mathfrak{V}'/W_n{}^0} d\tilde{\mu}_n(\tilde{F})\{\rho_n(\tilde{F}+g) \\ &\quad - \rho_n(\tilde{F})\,|a_g(\tilde{F})_n|^2\}\varphi_M(\tilde{F})\psi_M(\tilde{F}). \end{aligned} \tag{6.1}$$

Now we show that[30] for $g \in W_n$

$$\rho_n(\tilde{F}+g) \geq \rho_n(\tilde{F})\,|a_g(\tilde{F})_n|^2 \tag{6.2}$$

almost everywhere on $\mathfrak{V}'/W_n{}^0$. Indeed, let Δ be a cylinder set with arbitrary base $\tilde{\Delta} \subset \mathfrak{V}'/W_n{}^0$. Let $\chi_\Delta(F)$ be the characteristic function. Then the first term in the decomposition

$$\chi_\Delta(F)a_g(F) = \chi_\Delta(F)a_g(F)_n + \chi_\Delta(F)a_g(F)_{n^\perp}$$

lies in $\mathcal{H}_n$ since $\chi_\Delta \in \mathcal{H}_n$, while the second lies in $\mathcal{H}_{n^\perp}$ since for all $\varphi_n \in \mathcal{H}_n$ one has $\langle \varphi_n, \chi_n a_{gn^\perp} \rangle = \langle \varphi_n \chi_\Delta, a_{gn^\perp} \rangle = 0$. Hence $P_n(\chi_\Delta a_g) = \chi_\Delta a_{gn}$, and $\|P_n(\chi_\Delta a_g)\| \leq \|\chi_\Delta a_g\|$ just means

$$\begin{aligned} \int_{\tilde{\Delta}} d\tilde{\mu}_n(\tilde{F})\,|a_g(\tilde{F})_n|^2 &\leq \int_{\mathfrak{V}'} d\mu(F)\,|a_g(F)|^2\chi_\Delta(F) \\ &= \int_{\tilde{\Delta}} d\tilde{\mu}_n(F)\,\frac{\rho_n(\tilde{F}+g)}{\rho_n(\tilde{F})}. \end{aligned}$$

Since $\tilde{\Delta}$ is arbitrary, this implies Eq. (6.2).

Returning to Eq. (6.1), we take the absolute value of both sides. Let $|\varphi_M(F)|, |\psi_M(F)| \leq C$. Then Eq. (6.2) yields

$$\begin{aligned} |K_n| \leq c^2 \int_{W_n} d^n g \int_{\mathfrak{V}'/W_n{}^0} d\tilde{\mu}_n(\tilde{F}) \\ \times \{\rho_n(\tilde{F}+g) - \rho_n(\tilde{F})\,|a_g(\tilde{F})_n|^2\}. \end{aligned} \tag{6.3}$$

Using again Eq. (4.23), the right-hand side just becomes the expression of condition (d) if one puts $n = n_i$. Hence K_{n_i} tends to zero for $i \to \infty$. Then lemmas 4.5 and 4.6 immediately imply (c) for bounded functions of $\mathcal{H}_M$, $M = 1, 2, \cdots$.

These functions are dense in each $\mathcal{H}_M$ and hence dense in $\mathcal{H}$. Let φ, ψ be arbitrary vectors of $\mathcal{H}$. One can assume $\|\varphi\| = \|\psi\| = 1$. Let $1 \geq \epsilon > 0$. There exist an M and bounded functions $\varphi_M(F)$, $\psi_M(F) \in \mathcal{H}_M$ such that $\|\varphi_M\|$, $\|\psi_M\| \leq 1$ and $\|\varphi - \varphi_M\| < \epsilon/5$, $\|\psi - \psi_M\| < \epsilon/5$. Then, as in Eqs. (4.26) and (4.27), it follows that

$$\overline{\lim_i} |I_{n_i}(\varphi, \varphi_0, \psi) - \langle \varphi, \psi \rangle| < \epsilon.$$

(c) → (b) → (a): The first implication follows from $|I_n(\varphi, \varphi_0, \varphi)| \leq \|\varphi\|^2$, and the second is trivial.

Q.E.D.

The above theorem is relatively strong. For not only does $\overline{\lim} I_n(\varphi_0, \varphi_0, \varphi_0) = 1$ imply

$$\overline{\lim} I_n(\varphi, \varphi_0, \varphi) = \|\varphi\|^2$$

[30] This will turn out to be a decisive point for this section because it means that the term in curly brackets on the right-hand side of Eq. (6.1) remains unaffected when taking absolute values.

for all $\varphi \in \mathcal{H}$, but also the surprising fact follows that there exists a subsequence n_i, the same for all vectors, such that the limit superior can be replaced by a limit. Normally, one would have expected this subsequence to depend on φ. In Paper II the class of all representations satisfying the above conditions will be determined.

For the case of a simple limit, the proof of Theorem 6.1 immediately implies the following:

Corollary 6.1: Let the assumptions be as in Theorem 6.1, and let $n_1 < n_2 < \cdots$ be a sequence of natural numbers. Then the following statements are equivalent:

(a) $\lim_{i\to\infty} I_{n_i}(\varphi_0, \varphi_0, \varphi_0) = 1$;

(b) $\lim_{i\to\infty} I_{n_i}(\varphi, \varphi_0, \psi) = \langle \varphi, \psi \rangle$, for all $\varphi, \psi \in \mathcal{H}$;

(c) $\lim_{i\to\infty} \int_{W_{n_i}} d^{n_i}g \int_{\mathfrak{U}'} d\mu(F) \times \rho_{n_i}(F)\{|a_g(F)|^2 - |a_g(F)_{n_i}|^2\} = 0.$

Now we turn to the case $\sup \overline{\lim}$, where the supremum is taken with respect to all bases of $\mathfrak{U}$. We will find the same phenomenon as in Theorem 6.1. Firstly, it suffices that Eq. (2.36) holds for φ_0; secondly, there exists a fixed sequence of bases such that for all $\varphi \in \mathcal{H}$ the supremum can be replaced by an ordinary limit. This will be proved in the next theorem. In Theorem 6.3 it will be shown that one can even replace $\sup_\beta \overline{\lim}_n$ by an ordinary limit over a kind of diagonal sequence, which allows the transition to scalar products.

If $h_1^\beta, h_2^\beta, \cdots$ is a basis of $\mathfrak{U}$, W_n^β is defined as in Eq. (2.36) by $W_n^\beta = \{h_1^\beta, \cdots, h_n^\beta\}$. Define $\rho_n^\beta(F)$, $\mathcal{H}_n^\beta$, $a_g(F)_n^\beta$, $I_n^\beta(\varphi, \varphi_0, \psi)$ by means of W_n^β in the same way as ρ_n, $\mathcal{H}_n$, $a_g(F)_n$, $I_n(\varphi, \varphi_0, \psi)$ in Sec. 4.

Theorem 6.2: Let $U(f, g)$ be a representation of the CCR, and let the unit vector φ_0 be cyclic for $U(f)$ in such a way that, for any dense linear subspace $\mathfrak{U}_0$ of $\mathfrak{U}$, φ_0 is already cyclic for $U(\mathfrak{U}_0)$. Then the following statements are equivalent:

(a) $\sup_\beta \overline{\lim}_n I_n^\beta(\varphi_0, \varphi_0, \varphi_0) = 1$;

(b) $\sup_\beta \overline{\lim}_n I_n^\beta(\varphi, \varphi_0, \varphi) = \|\varphi\|^2$, for all $\varphi \in \mathcal{H}$;

(c) There exists a sequence of bases $(h_1^{(\nu)}, h_2^{(\nu)}, \cdots)$, $\nu = 1, 2, \cdots$, such that for all $\varphi \in \mathcal{H}$

$$\lim_{\nu\to\infty} \overline{\lim_{n\to\infty}} I_n^{(\nu)}(\varphi, \varphi_0, \varphi) = \|\varphi\|^2;$$

(d) $\inf_\beta \overline{\lim_n} \int_{W_n{}^\beta} d^n g \int_{\mathfrak{U}'} d\mu(F) \times \rho_n^\beta(F)\{|a_g(F)|^2 - |a_g(F)_n^\beta|^2\} = 0.$

The proof will yield the following:

Corollary 6.2: Let $(h_1^{(\nu)}, h_2^{(\nu)}, \cdots)$, $\nu = 1, 2, \cdots$, be a sequence of bases of $\mathfrak{U}$ and let the unit vector φ_0 be cyclic for every $U(\mathfrak{U}_0^{(\nu)})$, where $\mathfrak{U}_0^{(\nu)}$ consists of all finite linear combinations of $h_1^{(\nu)}, h_2^{(\nu)}, \cdots$. Then the following statements are equivalent:

(a) $\lim_\nu \overline{\lim_n} I_n^{(\nu)}(\varphi_0, \varphi_0, \varphi_0) = 1$;

(b) $\lim_\nu \overline{\lim_n} I_n^{(\nu)}(\varphi, \varphi_0, \psi) = \|\varphi\|^2$, for all $\varphi \in \mathcal{H}$;

(c) $\lim_\nu \overline{\lim_n} \int_{W_n{}^{(\nu)}} d^n g \int_{\mathfrak{U}'} d\mu(F) \times \rho_n^{(\nu)}(F)\{|a_g(F)|^2 - |a_g(F)_n^{(\nu)}|^2\} = 0.$

First we show the following simple lemma:

Lemma 6.1: Let $\varphi(F) \in L_\mu^2 \triangleq \mathcal{H}$ with $|\varphi(F)| \leq c < \infty$. Then for any $\epsilon > 0$, any β and any $\eta > 0$, there exist an M and a $\varphi_M(F) \in \mathcal{H}_M^\beta$ such that $|\varphi_M(F)| \leq c + \eta$ and $\|\varphi - \varphi_M\| < \epsilon$.

Proof: For each β one has $\mathcal{H} = \{\overline{\bigcup_n \mathcal{H}_n^\beta}\}$, by assumption of the above theorem. Choose $\epsilon_1 > 0$ such that $\epsilon_1^2 + \epsilon_1 c^2/\eta = \epsilon^2$. Then for each β there exist an M and a $\tilde{\varphi}_M(F) \in \mathcal{H}_M^\beta$ such that $\|\tilde{\varphi}_M - \varphi\| \leq \epsilon_1$. Schwarz's inequality and the finiteness of μ imply

$$\begin{aligned} \epsilon_1^2 &\geq \left\{\int d\mu\, |\tilde{\varphi}_M(F) - \varphi(F)|^2\right\} \cdot \left\{\int d\mu \cdot 1\right\} \\ &\geq \left\{\int d\mu\, |\tilde{\varphi}_M(F) - \varphi(F)|\right\}^2 \\ &\geq \left\{\int d\mu\, ||\tilde{\varphi}_M(F)| - |\varphi(F)||\right\}^2. \end{aligned} \tag{6.4}$$

Let $\Delta \equiv \{F \in \mathfrak{U}' : |\varphi_M(F)| > c + \eta\}$ and let $W_M^{\beta 0}$ be the annihilator of W_M^β in $\mathfrak{U}'$. Since $\tilde{\varphi}_M(F)$ is constant within each coset $F + W_M^{\beta 0}$, the characteristic function $\chi_\Delta(F)$ lies in $\mathcal{H}_M^\beta$. Equation (6.4) implies

$$\epsilon_1 \geq \int_\Delta d\mu\{|\tilde{\varphi}_M(F) - |\varphi(F)|\} \geq \eta \int_\Delta d\mu = \eta\mu(\Delta). \tag{6.5}$$

Put $\varphi_M(F) \equiv \tilde{\varphi}_M(F) \cdot (1 - \chi_\Delta(F))$. Then $\varphi_M(F) \in \mathcal{H}_M^\beta$, $|\varphi_M(F)| \leq c + \eta$, and

$$\begin{aligned} \|\varphi_M - \varphi\|^2 &= \int_{\mathfrak{U}'-\Delta} d\mu\, |\tilde{\varphi}_M - \varphi|^2 + \int_\Delta d\mu\, |\varphi|^2 \\ &\leq \epsilon_1^2 + c^2 \cdot \mu(\Delta) \\ &\leq \epsilon_1^2 + c^2\epsilon_1/\eta = \epsilon^2. \end{aligned} \quad \text{Q.E.D.} \tag{6.6}$$

Proof of Theorem 6.2: We show (a) $\leftrightarrow$ (d) $\rightarrow$ (c) $\rightarrow$ (b) $\rightarrow$ (a).

(a) $\leftrightarrow$ (d): According to lemmas 4.5 and 4.6, (d) is just another form of (a).

(d) $\rightarrow$ (c): There is a sequence of bases $(h_1^{(\nu)}, h_2^{(\nu)}, \cdots)$, $\nu = 1, 2, \cdots$, such that the supremum in (a) can be replaced by a limit:

$$\text{(a')} \qquad \lim_{\nu} \overline{\lim_{n}}\, I_n^{(\nu)}(\varphi_0, \varphi_0, \varphi_0) = 1.$$

Conversely, (a') implies (a) by Eq. (2.31). An equivalent form of (a') is

$$\text{(d')} \quad \lim_{\nu} \overline{\lim_{n}} \int_{W_n^{(\nu)}} d^n g \int_{\mathfrak{V}'} d\mu \times \rho_n^{(\nu)}(F)\{|a_g(F)|^2 - |a_g(F)_n^{(\nu)}|^2\} = 0.$$

We now show that (a') and (d') imply (c). First let $\varphi(F) \in L_\mu^2 \triangleq \mathcal{H}$ be bounded, $|\varphi(F)| \leq c$, say. One can assume $\|\varphi\| = 1$. Let $1 \geq \epsilon > 0$. We have to show that there is a $\nu_0 = \nu_0(\epsilon)$ such that for $\nu \geq \nu_0$

$$0 \leq 1 - \overline{\lim_{n}}\, I_n^{(\nu)}(\varphi, \varphi_0, \varphi) \leq \epsilon. \tag{6.7}$$

For each ν there is, by the above lemma, an $M = M(\nu)$ and a $\varphi_M^{(\nu)}(F) \in \mathcal{H}_M^{(\nu)}$ such that $|\varphi_M^{(\nu)}(F)| \leq 2c$, $\|\varphi_M^{(\nu)}\| \leq 1$, and $\|\varphi - \varphi_M^{(\nu)}\| < \epsilon/4$. Due to linearity and Eq. (2.31), one obtains, in a similar way as Eq. (4.26), that

$$|I_n^{\beta}(\varphi, \varphi_0, \varphi) - I_n^{\beta}(\varphi_M^{(\nu)}, \varphi_0, \varphi_M^{(\nu)})| \leq \tfrac{3}{4}\epsilon \tag{6.8}$$

for all β, n. This implies

$$\left| \overline{\lim_{n}}\, I_n^{\beta}(\varphi, \varphi_0, \varphi) - \overline{\lim_{n}}\, I_n^{\beta}(\varphi_M^{(\nu)}, \varphi_0, \varphi_M^{(\nu)}) \right| \leq \tfrac{3}{4}\epsilon. \tag{6.9}$$

Define ϵ_ν by

$$\overline{\lim_{n}}\, I_n^{(\nu)}(\varphi_0, \varphi_0, \varphi_0) \equiv 1 - \epsilon_\nu. \tag{6.10}$$

Then $\epsilon_\nu \geq 0$ and $\lim_\nu \epsilon_\nu = 0$. Hence there is a $\tilde{\nu}_0$ such that $0 \leq \epsilon_\nu \leq \epsilon/16c^2$ for all $\nu \geq \tilde{\nu}_0$. Choose $\nu_0 = \tilde{\nu}_0$. One has

$$\begin{aligned} 0 &\leq 1 - \overline{\lim_{n}}\, I_n^{(\nu)}(\varphi, \varphi_0, \varphi) \\ &= 1 - \overline{\lim_{n}}\, I_n^{(\nu)}(\varphi_M^{(\nu)}, \varphi_0, \varphi_M^{(\nu)}) \\ &\quad + \overline{\lim_{n}}\, I_n^{(\nu)}(\varphi_M^{(\nu)}, \varphi_0, \varphi_M^{(\nu)}) - \overline{\lim_{n}}\, I_n^{(\nu)}(\varphi, \varphi_0, \varphi) \\ &\leq \tfrac{3}{4}\epsilon + 1 - \overline{\lim_{n}}\, I_n^{(\nu)}(\varphi_M^{(\nu)}, \varphi_0, \varphi_M^{(\nu)}). \end{aligned} \tag{6.11}$$

By the same argument as in Eqs. (4.1)–(4.3), one obtains for $n \geq M$

$$\begin{aligned} &1 - I_n^{(\nu)}(\varphi_M^{(\nu)}, \varphi_0, \varphi_M^{(\nu)}) \\ &\quad \leq 4c^2 \int_{W_n^{(\nu)}} d^n g \int_{\mathfrak{V}'} d\mu \rho_n^{(\nu)}(F)\{|a_g(F)|^2 - |a_g(F)_n^{(\nu)}|^2\} \\ &\quad = 4c^2(1 - I_n^{(\nu)}(\varphi_0, \varphi_0, \varphi_0)). \end{aligned} \tag{6.12}$$

Hence the right-hand side of Eq. (6.11) is smaller than $\frac{3}{4}\epsilon + 4c^2\epsilon\nu \leq \frac{3}{4}\epsilon + \frac{1}{4}\epsilon = \epsilon$ for $\nu \geq \nu_0$. This proves Eq. (6.7), and thus (c), for bounded functions. Since these are dense in $L_\mu^2 \triangleq \mathcal{H}$, the validity of (c) for all elements of $\mathcal{H}$ follows by the same argument as in Eqs. (4.26) and (4.27).

(c) $\rightarrow$ (b) $\rightarrow$ (a): The first implication follows from Eq. (2.31), and the second is trivial. Q.E.D.

In condition (c) of the above theorem the supremum is replaced by a limit, but there still appears the limit superior. The natural question is whether this can also be replaced by a limit over a subsequence which is independent of φ. For φ_0 there exists, of course, such a subsequence. It is, however, uncertain if there exists a limit with this subsequence for $I_n^{(\nu)}(\varphi_M^{(\nu)}, \varphi_0, \varphi_M^{(\nu)})$ in Eq. (6.12). If one could prove the existence of this limit, everything would go through as before. Equation (6.12) only shows that, instead of $\overline{\lim}_n$, one may take any other limit point. This means that one just has to go sufficiently far in the sequence and that the actual limit point, i.e., $\overline{\lim}_n$ or another one, does not matter because their difference is restricted anyway. This remark makes it seem likely that one can find a kind of diagonal sequence such that $\lim_\nu \overline{\lim}_n$, which is a sort of double limit, can be replaced by an ordinary single limit. This is indeed the case.

Theorem 6.3: Let the assumptions be as in Theorem 6.2, and let

$$\sup_{\beta} \overline{\lim_{n}}\, I_n^{\beta}(\varphi_0, \varphi_0, \varphi_0) = 1. \tag{6.13}$$

Or, somewhat weaker, let the assumptions be as in Corollary 6.2, and let[31]

$$\lim_{\nu} \overline{\lim_{n}}\, I_n^{(\nu)}(\varphi_0, \varphi_0, \varphi_0) = 1. \tag{6.14}$$

Then there exists for each ν an index $n = n(\nu)$ such that for all $\varphi, \psi \in \mathcal{H}$

$$\lim_{\nu \to \infty} I_{n(\nu)}^{(\nu)}(\varphi, \varphi_0, \psi) = \langle \varphi, \psi \rangle. \tag{6.15}$$

Proof: The above cyclicity assumption implies that $\mathcal{H}$ is separable.[32] Let $\varphi_1, \varphi_2, \cdots$ be a denumerable dense set in $\mathcal{H}$, and let $P_n^{(\nu)}$ be the projection operator onto $\mathcal{H}_n^{(\nu)}$. For each ν, $P_n^{(\nu)}$ converges strongly to $\mathbf{1}$ for $n \to \infty$ by lemma 4.1. Hence for each ν there is an index $m(\nu)$ such that $\|P_{m(\nu)}^{(\nu)}\varphi_i - \varphi_i\| < \nu^{-1}$ for $i = 1, \cdots, \nu$. Let φ be any vector in $\mathcal{H}$, and let $\epsilon > 0$. There exists an index i_0 such that $\|\varphi_{i_0} - \varphi\| < \epsilon/3$,

[31] Obviously Eq. (6.13) implies Eq. (6.14).

[32] This simple fact is easily shown directly. It also follows from a lemma in Paper II, Sec. 5 (J. Math. Phys., to be published).

and for $\nu \geq i_0$, $\epsilon/3$ one has

$$\|P^{(\nu)}_{m(\nu)}\varphi - \varphi\| \leq \|P^{(\nu)}_{m(\nu)}(\varphi - \varphi_{i_0})\| + \|P^{(\nu)}_{m(\nu)}\varphi_{i_0} - \varphi_{i_0}\| + \|\varphi_{i_0} - \varphi\| \leq \epsilon. \quad (6.16)$$

Hence $P^{(\nu)}_{m(\nu)} \to \mathbf{1}$ strongly for $\nu \to \infty$.

Let ϵ_ν be defined by Eq. (6.10), and for each ν choose an index $n(\nu)$ such that $n(\nu) \geq m(\nu)$ and

$$1 - I^{(\nu)}_{n(\nu)}(\varphi_0, \varphi_0, \varphi_0) \leq 2\epsilon_\nu.$$

Now let $\varphi(F)$, $\psi(F)$ be any two bounded functions in L^2_μ, $|\varphi(F)| \leq c$, and $|\psi(F)| \leq c < \infty$ say, and let $\epsilon > 0$. We can assume $\|\varphi\| = \|\psi\| = 1$. Put $\epsilon' \equiv \epsilon/10$. Then there is a ν_0 such that for $\nu \geq \nu_0$ one has $0 \leq \epsilon_\nu \leq \epsilon'/2c^2$, $\|\varphi - P^{(\nu)}_{m(\nu)}\| \leq \epsilon'/2$, and

$$\|\psi - P^{(\nu)}_{m(\nu)}\| \leq \epsilon'/2.$$

By the same argument as in the proof of lemma 6.1, it follows that for each $\nu \geq \nu_0$ there is a function $\varphi^{(\nu)}_{m(\nu)} \in \mathfrak{K}^{(\nu)}_{m(\nu)}$ such that $|\varphi^{(\nu)}_{m(\nu)}(F)| \leq 2c$, $\|\varphi^{(\nu)}_{m(\nu)}\| \leq 1$, and $\|\varphi - \varphi^{(\nu)}_{m(\nu)}\| \leq \epsilon'$. The same holds for ψ. Then for $\nu \geq \nu_0$

$$\begin{aligned} |I^{(\nu)}_{n(\nu)}(\varphi, \varphi_0, \psi) - \langle\varphi, \psi\rangle| &\leq |I^{(\nu)}_{n(\nu)}(\varphi, \varphi_0, \psi) - I^{(\nu)}_{n(\nu)}(\varphi^{(\nu)}_{m(\nu)}, \varphi_0, \psi^{(\nu)}_{m(\nu)})| \\ &\quad + |I^{(\nu)}_{n(\nu)}(\varphi^{(\nu)}_{m(\nu)}, \varphi_0, \psi^{(\nu)}_{m(\nu)}) - \langle\varphi^{(\nu)}_{m(\nu)}, \psi^{(\nu)}_{m(\nu)}\rangle| \\ &\quad + |\langle\varphi^{(\nu)}_{m(\nu)}, \psi^{(\nu)}_{m(\nu)}\rangle - \langle\varphi, \psi\rangle|. \end{aligned} \quad (6.17)$$

The first term on the right-hand side is not greater than $3\epsilon'$ by Eq. (4.26), and the third not greater than $2\epsilon'$. For the second term, similar to Eqs. (6.12) and (6.1)–(6.3), one has

$$\begin{aligned} |I^{(\nu)}_{n(\nu)}(\varphi^{(\nu)}_{m(\nu)}, \varphi_0, \psi^{(\nu)}_{m(\nu)}) - \langle\varphi^{(\nu)}_{m(\nu)}, \psi^{(\nu)}_{m(\nu)}\rangle| &= \left| \int_{W_{n(\nu)^{(\nu)}}} d^n g \int_{\mathfrak{U}'} d\mu \right. \\ &\quad \left. \times \rho^{(\nu)}_n(F)\{|a_g(F)|^2 - |a_g(F)^{(\nu)}_n|^2\}\bar{\varphi}^{(\nu)}_{m(\nu)}\psi^{(\nu)}_{m(\nu)} \right| \\ &\leq 4c^2(1 - I^{(\nu)}_{n(\nu)}(\varphi_0, \varphi_0, \varphi_0)) \leq 8c^2\epsilon_\nu. \end{aligned} \quad (6.18)$$

Hence the left-hand side of Eq. (6.17) is smaller than ϵ for $\nu \geq \nu_0$. Q.E.D.

Up to now φ_0 has always been assumed to be cyclic. In Paper II it will be shown that under certain not very strong conditions the validity of Eqs. (2.33), (2.35), or (2.36) for some φ_0 implies the validity for any other unit vector. It will also turn out that in this case Eq. (2.30) of lemma 2.1 can be generalized to infinitely many degrees of freedom, the corresponding limit being $\langle\psi_1, \psi_2\rangle\langle\varphi_2, \varphi_1\rangle$.

One can also apply the methods of Sec. 4 to these questions, but the treatment in Paper II seems to be simpler.

7. DISCUSSION AND A COUNTEREXAMPLE

The integral conditions (4.25) of Theorem 4.1, (d) of Theorem 6.1, (d) of Theorem 6.2, and (c) of corollary 6.2 specify the kind of convergence of the projections $a_g(F)_n$ towards $a_g(F)$. Of course, one now can formulate numerous sufficient conditions which imply this kind of convergence. The particularly simple condition $a_g(F)_{n_i} = a_g(F)$ has been used in Sec. 5 for PTPR.

One immediately gets the natural idea that stronger continuity properties of the representation might lead to the required kind of convergence. For instance, one could choose the space S of Schwarz for $\mathfrak{U}$ and demand continuity of the representation with respect to the usual topology of S. Since S is a nuclear space in this topology, $\mathfrak{U}'$ can be replaced[19] by the considerably smaller space S'. Thus one might try to exploit the far-reaching results of the theory of nuclear spaces and of rigged Hilbert spaces.[19]

In general, however, this hope is unfounded. Below, a relatively simple example of a representation will be given in which $U(f)$ is cyclic and for which a kernel integral formula holds neither with a limit superior nor with a supremum over all bases, although the representation is continuous in the topology of S. The existence of such a representation can be deduced from general reasons. In Part II we are going to show that every representation fulfilling a kernel integral formula has to be irreducible. And since there are representations with $\mathfrak{U} = S$ which are cyclic with respect to $U(f)$ and continuous in the topology of S but not irreducible, a kernel integral formula cannot hold for such representations. Since the example is quite instructive and does not make use of the general theory, it may be worthwhile to show this fact directly.

Consider[33] the direct sum of two representations which are given by the vacuum functionals

$$E_j(f, g) = e^{-\frac{1}{4}\{(m_j(f,f)+m_j^{-1}(g,g)\}-i/2(f,g)}, \quad j = 1, 2; \quad m_1 > m_2 > 0, \quad (7.1)$$

in Hilbert spaces $\mathfrak{K}_1$ and $\mathfrak{K}_2$. In $\mathfrak{K} = \mathfrak{K}_1 \oplus \mathfrak{K}_2$ we choose as "vacuum state"

$$|0\rangle = 2^{-\frac{1}{2}}\{|0\rangle_1 \oplus |0\rangle_2\}, \quad (7.2)$$

where $|0\rangle_1$, $|0\rangle_2$ are the vacuum states for E_1, E_2. The representations determined by E_1 and E_2 are inequivalent and irreducible, and $|0\rangle_i$ is cyclic with respect to the field. They are tensor-product representations.[3,11] If one takes S as test-function space, the representations are continuous in the topology of $S \times S$.

[33] This example was suggested to the author by J. R. Klauder.

Denote by $U_i(f, g)$ the operators in $\mathcal{H}_i$. Then in $\mathcal{H}$, $U(f, g) = U_1(f, g) \oplus U_2(f, g)$, and with $|0\rangle$ one obtains as vacuum functional

$$E(f, g) = \tfrac{1}{2}\{E_1(f, g) + E_2(f, g)\}. \tag{7.3}$$

Before proving that $|0\rangle$ is cyclic for $U(f)$, we show that E fulfills neither condition (a) of Theorem 6.1 nor the corresponding condition (a) of Theorem 6.2. For any basis $h_1, h_2, \cdots$ of S, one has

$$\int_{W_n \times W_n} d^n f\, d^n g/(2\pi)^n\, |E(f, g)|^2$$

$$= \int_{W_n \times W_n} d^n f\, d^n g/(2\pi)^n \{\tfrac{1}{4}\,|E_1|^2 + \tfrac{1}{4}\,|E_2|^2 + \tfrac{1}{2}\,|E_1 E_2|\}. \tag{7.4}$$

By means of the well-known formula

$$(2\pi)^{-n/2} \int \exp\{-a/2\mathbf{x}^2\}\, d^n\mathbf{x} = a^{-n/2} \quad (a > 0),$$

one obtains for the first integral $\frac{1}{2}$ and for the second $\{\frac{1}{2} + \frac{1}{4}(m_1/m_2 + m_2/m_1)\}^{-n/2}$, which tends to zero for $n \to \infty$ and $m_1 \neq m_2$. Hence for any basis of S the left-hand side of Eq. (7.4) tends to $\frac{1}{2}$ for $n \to \infty$.

It remains to show that $|0\rangle$ is cyclic for $U(f)$. This is achieved by means of the cluster decomposition property[34] of the representations E_i. If one defines $f_a(x) \equiv f(x - a)$ and the translation operators $T_i(a)$ by $T_i(a)\,|f, g\rangle_i \equiv |f_a, g_a\rangle_i$, then, according to this property, $T_i(a)$ converges weakly to the projection operator $|0\rangle_{i\,i}\langle 0|$ for $|a| \to \infty$. Now assume that $|0\rangle$ is not cyclic for $U(f)$. Then there is a $|\psi\rangle = |\psi\rangle_1 \oplus |\psi\rangle_2 \in \mathcal{H}$ such that $|\psi\rangle \neq 0$ and $\langle\psi|\, U(f)\,|0\rangle = 0$ for all f. Thus $\langle\psi\,|f + y_a\rangle = 0$ for any function $y \in S$ and any a, hence also for $|a| \to \infty$. Evaluating this and using the definition of E_i, one obtains

$$e^{-m_1(y,y)/4}\,{}_1\langle\psi\,|f\rangle_1 + e^{-m_2(y,y)/4}\,{}_2\langle\psi\,|f\rangle_2 = 0. \tag{7.5}$$

Dividing by $\exp\{-m_2(y, y)/4\}$ and letting (y, y) tend towards ∞, it follows from $m_1 > m_2$ that ${}_2\langle\psi\,|f\rangle_2 = 0$. Hence also the remaining term in Eq. (7.5) has to vanish, i.e., ${}_1\langle\psi\,|f\rangle_1 = 0$. Because of the cyclicity of $|0\rangle_i$ with respect to $U_i(f)$, this implies $|\psi\rangle_1 = |\psi\rangle_2 = 0$, thus $|\psi\rangle = 0$, in contradiction to the assumption.

The above example provides a representation which is cyclic with respect to $U(f)$ but not irreducible. For finitely many degrees of freedom this cannot happen, and our proof would break down due to the missing cluster decomposition property. For $m_1 = m_2$ the integral in Eq. (7.4) assumes the correct value 1, but $|0\rangle$ is not cyclic in this case. For other vectors the kernel integral need not tend to the required value. Thus the cyclicity assumption in Theorems 6.1 and 6.2 is quite important. In Paper II it will be shown that this assumption can be replaced by an irreducibility condition.

ACKNOWLEDGMENTS

The author's thanks are due to Professor G. Ludwig for his generous encouragement. The author is indebted to Professor J. R. Klauder for several stimulating discussions. He would also like to thank Professor A. Salam and Professor P. Budini for the hospitality extended to him at the International Centre for Theoretical Physics, Trieste, where part of this work was done. Financial support of the Bundesministerium für Wissenschaftliche Forschung, Bonn, is gratefully acknowledged.

[34] The physical idea underlying the cluster decomposition property has been discussed by F. Coester and R. Haag, Phys. Rev. **117**, 1137 (1960).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Group Analysis of Maxwell's Equations

MOSHE CARMELI
General Physics Research Laboratory, Aerospace Research Laboratories, Wright-Patterson AFB, Ohio

(Received 17 February 1969)

In this paper we write down and solve Maxwell's equations without sources when the field variables are considered as functions over the group SU_2. A Hilbert space is then constructed out of the field functions. An expansion of the field functions in terms of the matrix elements of the irreducible representation of SU_2 is shown to reduce the problem of solving Maxwell's equations to that of solving one partial differential equation with two variables. A Fourier transform reduces this equation into an ordinary differential equation which is identical to the partial-wave equation obtained from the Schrödinger equation with zero potential. The analogy between the mathematical method used in this paper in relation to the group SU_2 and the Fourier transform in relation to the additive group of real numbers is pointed out.

1. INTRODUCTION

In this paper we write down and solve Maxwell's equations without sources when the field variables are considered as functions over the rotation group O_3 or its covering group SU_2. This means the independent variables of the field functions will be the elements $g \in O_3$ or $u \in SU_2$. The variable $u \in SU_2$ will not, however, take over the whole set of the four coordinates t, $\mathbf{x}$, but only two of them. Clearly the time t and the radial distance $r = |\mathbf{x}|$ are unchanged under rotations. Accordingly, the independent parameters of the field functions will be taken as t, r, and g, or equivalently t, r, and u. The variable $u \in SU_2$ will replace the usual spherical angles θ and ϕ. An additional degree of freedom is so added since $u \in SU_2$ depends on three variables (such as Euler's angles). The physical field functions can be obtained by setting the additional variable equal to zero.

By working with functions defined over the group SU_2, we will be able to apply some powerful mathematical methods known from the theory of representations of compact topological groups.

An easy method[1,2] to describe a definite quantity as a function of $u \in SU_2$ was given recently and a brief summary is given in Sec. 2 below for the vector fields case. In Sec. 3 we apply the method to Maxwell equations. In Sec. 4 we discuss the properties of the field functions written over the group SU_2. A Hilbert space is constructed out of these functions and, accordingly, any solution of Maxwell's equations can then be considered as a vector in that Hilbert space. Section 5 is devoted to the solution of Maxwell's equations. This problem is reduced to the solution of only one ordinary differential equation which is formally identical to the partial wave equation in potential scattering. The static solutions are then carried out explicitly.

2. PRELIMINARIES AND NOTATIONS

In this section we review the method of writing vector fields as functions of elements u of the group SU_2 (the group of all unitary matrices of order two and determinant unity). For more details see Refs. 1 and 2.

Let $\mathbf{V}(x)$ be a (complex) vector field. Instead of decomposing $\mathbf{V}$ in some fixed coordinate system, we decompose it with respect to a triad of orthonormal vectors at each point in space. The triad of vectors is chosen so that one vector is directed along the radial coordinate r and the other two vectors are perpendicular to it. The component of $\mathbf{V}$ along the vector directed along r is of course just V_r. The other two components will then be given as linear combinations of the spherical components V_ϕ and V_θ. Because of the arbitrariness of the direction of the two vectors which are normal to the one directed along r, a new angle is introduced which we denote by ϕ_2. The other two quantities that specify the vector field $\mathbf{V}$ are then given by

$$V_1 = V_\phi \cos\phi_2 + V_\theta \sin\phi_2,$$
$$V_2 = -V_\phi \sin\phi_2 + V_\theta \cos\phi_2. \tag{2.1}$$

Each one of the field functions V_r, V_1, and V_2 is a function of the angles ϕ, θ, and ϕ_2 for each value of t and r. For any value of the set of the variables ϕ, θ, and ϕ_2, we can associate a rotation $g \in O_3$, whose Euler's angles are $\frac{1}{2}\pi - \phi$, θ, and ϕ_2:

$$g = g(\tfrac{1}{2}\pi - \phi, \theta, \phi_2). \tag{2.2}$$

Accordingly, the functions V_r, V_1, and V_2 are functions of g (of course, they are also functions of t and r):

$$V_r = V_r(g), \quad V_{1,2} = V_{1,2}(g). \tag{2.3}$$

[1] M. Carmeli, J. Math. Phys. **10**, 569 (1969).
[2] I. M. Gel'fand and Z. Ya. Shapiro, Usp. Mat., Nauk **7**, 3 (1952) [English transl.: Am. Math. Soc. Transl. (2) **2**, 207 (1956)]; I. M. Gel'fand, R. A. Minlos, and Z. Ya. Shapiro, *Representations of the Rotation and Lorentz Groups and their Applications* (Pergamon Press, Inc., New York, 1963).

The quantities V_1 and V_2 are not convenient to work with since under rotations they get mixed up. We define, instead, the new functions

$$\begin{aligned}\eta_{\pm}(g) &= -2^{-\frac{1}{2}}[V_1(g) \pm iV_2(g)] \\ &= -2^{-\frac{1}{2}}[V_\phi \pm iV_\theta]e^{\mp i\phi_2}, \qquad (2.4)\\ \eta_0(g) &= V_r(g).\end{aligned}$$

Clearly $\eta_\pm$ and η_0 satisfy the requirement for a function over O_3 to satisfy,[3] i.e.,

$$\begin{aligned}\eta(\phi_1 + 2\pi, \theta, \phi_2) &= \eta(\phi_1, \theta, \phi_2),\\ \eta(\phi_1, \theta, \phi_2 + 2\pi) &= \eta(\phi_1, \theta, \phi_2). \qquad (2.5)\end{aligned}$$

The functions η's can also be considered as functions over the group SU_2,

$$\eta = \eta(u), \qquad (2.6)$$

where $u \in SU_2$. Euler's angles are again employed to describe the elements $u \in SU_2$,

$$u = \begin{pmatrix} \cos\frac{\theta}{2}\exp\left[\frac{i}{2}(\phi_1 + \phi_2)\right] & i\sin\frac{\theta}{2}\exp\left[-\frac{i}{2}(\phi_1 - \phi_2)\right] \\ i\sin\frac{\theta}{2}\exp\left[\frac{i}{2}(\phi_1 - \phi_2)\right] & \cos\frac{\theta}{2}\exp\left[-\frac{i}{2}(\phi_1 + \phi_2)\right] \end{pmatrix}. \qquad (2.7)$$

Clearly also, $\eta(u)$ satisfy the requirement for a function over SU_2 to satisfy, i.e.,[3]

$$\begin{aligned}\eta(\phi_1 + 4\pi, \theta, \phi_2) &= \eta(\phi_1, \theta, \phi_2),\\ \eta(\phi_1, \theta, \phi_2 + 4\pi) &= \eta(\phi_1, \theta, \phi_2), \qquad (2.8)\\ \eta(\phi_1 + 2\pi, \theta, \phi_2 + 2\pi) &= \eta(\phi_1, \theta, \phi_2).\end{aligned}$$

An additional property these functions have is that[1]

$$\begin{aligned}\eta_{\pm}(\gamma u) &= e^{\pm i\lambda}\eta_{\pm}(u),\\ \eta_0(\gamma u) &= \eta_0(u), \qquad (2.9)\end{aligned}$$

where γ is given by

$$\gamma = \begin{pmatrix} e^{-i\lambda/2} & 0 \\ 0 & e^{i\lambda/2} \end{pmatrix}. \qquad (2.10)$$

3. MAXWELL'S EQUATIONS

The Maxwell equations in free space are given by

$$\begin{aligned}&\nabla\cdot\mathbf{E} = 0, \quad \nabla\cdot\mathbf{B} = 0,\\ &\nabla\times\mathbf{E} = -\frac{\partial\mathbf{B}}{\partial t}, \qquad (3.1)\\ &\nabla\times\mathbf{B} = \frac{\partial\mathbf{E}}{\partial t}.\end{aligned}$$

Introducing the complex vector field

$$\mathbf{V} = \mathbf{E} + i\mathbf{B},$$

Maxwell's equations can then be written as

$$\nabla\cdot\mathbf{V} = 0, \qquad (3.2a)$$

$$\nabla\times\mathbf{V} - i\frac{\partial\mathbf{V}}{\partial t} = 0. \qquad (3.2b)$$

We decompose Eq. (3.2b) into its spherical components and form the following four complex scalar equations out of them and of Eq. (3.2a):

$$\nabla\cdot\mathbf{V} \pm i\left\{\nabla\times\mathbf{V} - i\frac{\partial\mathbf{V}}{\partial t}\right\}_r = 0, \qquad (3.3a)$$

$$\left\{\nabla\times\mathbf{V} - i\frac{\partial\mathbf{V}}{\partial t}\right\}_\phi \pm i\left\{\nabla\times\mathbf{V} - i\frac{\partial\mathbf{V}}{\partial t}\right\}_\theta = 0. \qquad (3.3b)$$

Substituting now the expression for the symbol ∇ in Eqs. (3.3), we obtain

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2V_r) \pm \frac{\partial V_r}{\partial t} \pm \frac{1}{r\sin\theta} \times\left\{\left(i\cos\theta + i\sin\theta\frac{\partial}{\partial\theta} \pm \frac{\partial}{\partial\phi}\right)(V_\phi \mp iV_\theta)\right\} = 0, \qquad (3.4a)$$

$$\frac{1}{r}\left\{\mp\frac{\partial}{\partial r}[r(V_\phi \pm iV_\theta)] + \left(i\frac{\partial}{\partial\theta} \pm \operatorname{cosec}\theta\frac{\partial}{\partial\phi}\right)V_r\right\} - \frac{\partial}{\partial t}(V_\phi \pm iV_\theta) = 0. \qquad (3.4b)$$

To write Eqs. (3.4) over the group SU_2 we substitute for ϕ its value in terms of one of Euler's angles, $\phi = \frac{1}{2}\pi - \phi_1$. Accordingly, the derivatives $\partial/\partial\phi$ in Eqs. (3.4) should be replaced by $-\partial/\partial\phi_1$. Also, we use the notation

$$\begin{aligned}V_\pm &= -2^{-\frac{1}{2}}(V_\phi \pm iV_\theta),\\ V_0 &= V_r. \qquad (3.5)\end{aligned}$$

Equations (3.4) will then have the form

$$\frac{1}{r}\frac{\partial}{\partial r}(r^2V_0) \pm r\frac{\partial V_0}{\partial t} \mp 2^{\frac{1}{2}}\left(i\cot\theta + i\frac{\partial}{\partial\theta} \mp \operatorname{cosec}\theta\frac{\partial}{\partial\phi_1}\right)V_\mp = 0, \qquad (3.6a)$$

$$\pm\frac{\partial}{\partial r}(2^{\frac{1}{2}}rV_\pm) + \left(i\frac{\partial}{\partial\theta} \mp \operatorname{cosec}\theta\frac{\partial}{\partial\phi_1}\right)V_0 + 2^{\frac{1}{2}}r\frac{\partial}{\partial t}V_\pm = 0. \qquad (3.6b)$$

[3] M. A. Naimark, *Linear Representations of the Lorentz Group* (Pergamon Press, Inc., New York, 1964).

Denoting now

$$\eta_{\pm}(u) = V_{\pm}e^{\mp i\phi_2},$$
$$\eta_0(u) = V_0, \tag{3.7}$$

and introducing the operators

$$K_{\pm} = e^{\mp i\phi_2}\left(\pm\cot\theta\frac{\partial}{\partial\phi_2} + i\frac{\partial}{\partial\theta} \mp \operatorname{cosec}\theta\frac{\partial}{\partial\phi_1}\right),$$
$$K_3 = i\frac{\partial}{\partial\phi_2}, \tag{3.8}$$

Eqs. (3.6) now have the form

$$\frac{1}{2^{\frac{1}{2}}}\frac{1}{r}\left(\frac{\partial}{\partial r} \pm \frac{\partial}{\partial t}\right)(r^2\eta_0) \mp K_{\pm}\eta_{\mp} = 0,$$
$$\left(\pm\frac{\partial}{\partial r} + \frac{\partial}{\partial t}\right)(r\eta_{\pm}) + \frac{1}{2^{\frac{1}{2}}}K_{\pm}\eta_0 = 0. \tag{3.9}$$

Equations (3.9) are Maxwell's equations written partially over the group SU_2. The functions η's are functions of the coordinates t and r, and of course of $u \in SU_2$. The operators $K_{\pm}$ and K_3 are well known from the theory of representations of SU_2. They satisfy the following relations[4]:

$$K_{\pm}T^j_{mn} = [(j \pm m + 1)(j \mp m)]^{\frac{1}{2}}T^j_{m\pm1,n},$$
$$K_3T^j_{mn} = mT^j_{mn}, \tag{3.10}$$

where $T^j_{mn}(u)$ are the matrix elements of the irreducible representation of weight j of the group SU_2.

4. THE η FUNCTIONS

We will assume that the functions η's (i.e., $\eta_{\pm}$ and η_0 introduced in the last section) are such that their modulus squares are integrable with respect to du:

$$\int|\eta(u)|^2\,du < \infty. \tag{4.1}$$

The integral in Eq. (4.1) is an invariant integral[3,5] of the function $\eta(u)$ over the group SU_2. When Euler's angles are used to describe the three variables of u, the function $\eta(u)$ means simply a function of ϕ_1, θ, and ϕ_2, and du is an abbreviation for

$$du = \tfrac{1}{16}\pi^{-2}\sin\theta\,d\phi_1\,d\theta\,d\phi_2,$$

which satisfies

$$\int du = 1.$$

An important property of the invariant integral is that

$$\int\eta(uu_1)\,du = \int\eta(u_1u)\,du = \int\eta(u)\,du$$

for any $u_1 \in SU_2$, and

$$\int f(u^{-1})\,du = \int f(u)\,du.$$

As a consequence of the assumption (4.1), each $\eta(u)$ can be expanded in the form

$$\eta(t, r, u) = \sum_{j=0}^{\infty}\sum_{m,n=-j}^{j}\alpha^j_{mn}(t, r)T^j_{mn}(u), \tag{4.2}$$

where

$$\alpha^j_{mn}(t, r) = (2j + 1)A^j_{mn}(t, r), \tag{4.3}$$

$$A^j_{mn}(t, r) = \int\eta(t, r, u)T^{j*}_{mn}(u)\,du. \tag{4.4}$$

In Eqs. (4.2) and (4.4) $T^j_{mn}(u)$ are the matrix elements of the irreducible representation of SU_2. They satisfy the following orthogonality relation:

$$\int T^j_{mn}(u)T^{j'*}_{m'n'}(u)\,du = (2j + 1)^{-1}\delta_{jj'}\delta_{mm'}\delta_{nn'}.$$

The expression given above in terms of the elements of the matrix $T^j_{mn}(u)$ is analogous to that of the Fourier transform. The well-known Plancherel's formula for the Fourier transform will have the form

$$\int|\eta(u)|^2\,du = \sum_j(2j + 1)\sum_{m,n}|A^j_{mn}|^2 \tag{4.5}$$

in the present case. Just as the usual Fourier transform realizes a decomposition of the regular representation of the additive group of real numbers into its irreducible representations, the generalized Fourier transform (4.4) realizes an isometric mapping of the regular representation of SU_2 onto the direct sum of irreducible representations $u \to T^j(u)$, where each representation $u \to T^j(u)$ is included in this direct sum $2j + 1$ times. An analogous proposition and a formula similar to Eq. (4.5) hold for any compact topological group.[3,6,7]

For the particular function $\eta_{\pm}$ and η_0, we will have expansions similar to that of Eq. (4.2) with m now a fixed number[1]

$$\eta_{\pm}(t, r, u) = \sum_{j=1}^{\infty}\sum_{n=-j}^{j}\alpha^j_{\pm1,n}(t, r)T^j_{\pm1,n}(u), \tag{4.6}$$

$$\eta_0(t, r, u) = \sum_{j=0}^{\infty}\sum_{n=-j}^{j}\alpha^j_{0,n}(t, r)T^j_{0,n}(u). \tag{4.7}$$

[4] The operators K_+, K_-, and K_3, and Eqs. (3.10) are obtained from the usual operators and formulas by exchanging the roles of ϕ_1 and ϕ_2 and the fact that $T^j_{mn}(\phi_1, \theta, \phi_2) = T^j_{nm}(\phi_2, \theta, \phi_1)$. See, for example, Footnote 17 of Ref. 1.

[5] A. Weil, Actualities Sci. Ind., No. 869 (1938).

[6] L. S. Pontrjagin, *Topological Groups* (Princeton University Press, Princeton, N.J., 1946).

[7] M. A. Naimark, *Normed Rings* (P. Noordhoff Ltd., Groningen, The Netherlands, 1959).

Equations (4.6) and (4.7) are a direct result of the fact that $\eta_\pm$ and η_0 transform like $T^j_{\pm1,n}$ and $T^j_{0,n}$, respectively, under the transformation $u \to \gamma u$, where γ is given by Eq. (2.10).

We now discuss the space spanned by the functions $\eta_\pm$ and η_0.

Let us denote by $L^2(SU_2)$ the space of all measurable functions $\eta(u)$ satisfying the condition (4.1). This space is a complete Hilbert space where the scalar product is defined by

$$\langle \xi, \eta \rangle = \int \xi(u)\eta^*(u)\, du. \tag{4.8}$$

Following Naimark,[3] we denote by $L_2^{2s}(SU_2)$ the set of all functions $\phi_s(u) \in L^2(SU_2)$ satisfying the condition[8]

$$\phi_s(\gamma u) = e^{i\lambda s}\phi_s(u), \tag{4.9}$$

where the unitary matrix γ is given by Eq. (2.10). For each s, $s = 0, \pm\frac{1}{2}, \pm1, \cdots, L_2^{2s}(SU_2)$ is a Hilbert space which is a closed subspace of $L^2(SU_2)$ and so is complete. These subspaces are mutually orthogonal. This can easily be seen by calculating the scalar product $\langle \psi_r, \psi_s \rangle$. We have

$$\begin{aligned}\langle \psi_r, \psi_s \rangle &= \int \psi_r(u)\psi_s^*(u)\, du \\ &= \int \psi_r(\gamma u)\psi_s^*(\gamma u)\, du,\end{aligned} \tag{4.10}$$

because of the invariance property of the integral. Now,

$$\begin{aligned}\psi_r(\gamma u) &= e^{ir\lambda}\psi_r(u), \\ \psi_s(\gamma u) &= e^{is\lambda}\psi_s(u).\end{aligned} \tag{4.11}$$

Accordingly, we have

$$\langle \psi_r, \psi_s \rangle = e^{i(r-s)\lambda}\langle \psi_r, \psi_s \rangle. \tag{4.12}$$

This shows that $\langle \psi_r, \psi_s \rangle = 0$ if $r \neq s$.

We now form the orthogonal sum of the three subspaces $L_2^{2m}(SU_2)$, $m = -1, 0, 1$, which is obviously the space spanned by the functions η_-, η_0, η_+,

$$\mathcal{H} = L_2^{-2}(SU_2) \oplus L_2^0(SU_2) \oplus L_2^2(SU_2). \tag{4.13}$$

$\mathcal{H}$ is then the aggregate of all sums[9]

$$\eta(u) = \sum_{k=-1}^{1} \eta_k(u), \tag{4.14}$$

where $\eta_k \in L_2^{2k}(SU_2)$. The space $\mathcal{H}$ is a closed subspace of $L^2(SU_2)$. For any two functions $\xi, \eta \in \mathcal{H}$ we define a scalar product by

$$\langle \xi, \eta \rangle = \int \xi(u)\eta^*(u)\, du. \tag{4.15}$$

Using Eq. (4.14) and an analogous expression for ξ, and using Eq. (4.12), we obtain[10]

$$\langle \xi, \eta \rangle = \sum_{k=-1}^{1} \langle \xi_k, \eta_k \rangle. \tag{4.16}$$

One can easily verify that the above definition for the scalar product satisfies the usual requirements: (1) $\langle \xi, \eta \rangle^* = \langle \eta, \xi \rangle$; (2)

$$\langle \alpha\xi + \beta\eta, \psi \rangle = \alpha\langle \xi, \psi \rangle + \beta\langle \eta, \psi \rangle;$$

(3) $\langle \psi, \psi \rangle \geq 0$, $\langle \psi, \psi \rangle = 0$, if and only if $\psi = 0$, for any $\xi, \eta, \psi \in \mathcal{H}$, and any complex numbers α and β. Moreover, since each of the three subspaces $L_2^{2s}(SU_2)$, $s = -1, 0, 1$, is complete, $\mathcal{H}$ is complete. It thus follows that $\mathcal{H}$ is a complete Hilbert space.[11]

5. SOLUTION OF MAXWELL'S EQUATIONS

We now solve Eqs. (3.9) by assuming solutions of the form (4.6) and (4.7).[12] Using (4.6) and (4.7) in (3.9) and using Eq. (3.10), we obtain

$$\frac{1}{2^{\frac{1}{2}}}\frac{1}{r}\left(\frac{\partial}{\partial r} \pm \frac{\partial}{\partial t}\right)(r^2\alpha^j_{0,m}) \mp [j(j+1)]^{\frac{1}{2}}\alpha^j_{\mp1,m} = 0, \tag{5.1}$$

$$\left(\pm\frac{\partial}{\partial r} + \frac{\partial}{\partial t}\right)(r\alpha^j_{\pm1,m}) + \left[\frac{j(j+1)}{2}\right]^{\frac{1}{2}}\alpha^j_{0,m} = 0, \tag{5.2}$$

where $j = 1, 2, 3, \cdots$ for $\alpha^j_{\mp1,m}$ and $j = 0, 1, 2, 3, \cdots$ for $\alpha^j_{0,m}$, and $m = -j, -j+1, \cdots, j$ for both cases. (One can let $j = 0, 1, 2, \cdots$ for both cases with the understanding that $\alpha^j_{\pm1,m} = 0$ for $j = 0$.) By elimination we can get a separate partial differential equation for the $\alpha^j_{0,m}$, and expressing $\alpha^j_{\pm1,m}$ in terms of $\alpha^j_{0,m}$. We obtain

$$\left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial r^2}\right)(r^2\alpha^j_{0,m}) + j(j+1)\alpha^j_{0,m} = 0 \tag{5.3}$$

[8] We recall that the electromagnetic field functions $\eta_-(u)$, $\eta_0(u)$, and $\eta_+(u)$ satisfy Eq. (4.9) with values $s = -1, 0$, and 1, respectively [compare Eq. (2.9)]. Accordingly, $\eta_- \in L_2^{-2}(SU_2)$, $\eta_0 \in L_2^0(SU_2)$, and $\eta_+ \in L_2^2(SU_2)$.

[9] See, for example, Ref. 3.

[10] If we write the three field functions η_-, η_0, and η_+ as a row matrix and denote by $\eta\dagger$ its Hermitian conjugate, the scalar product in $\mathcal{H}$ can then be written as $\langle \xi, \eta \rangle = \int \xi\eta\dagger\, du$, where the integrand here is the product of the row matrix ξ and the column matrix $\eta\dagger$. It will be noted that this integrand is invariant under $\xi \to \xi U$, $\eta \to \eta U$, where U is a 3×3 unitary matrix.

[11] It is interesting to point out that an analogous Hilbert space can be constructed for the Weyl tensor of the gravitational field. See M. Carmeli, Phys. Letters **28A**, 683 (1969).

[12] Expansion in terms of matrix elements of the irreducible representations of the rotation group in which the Euler angles are employed with $\phi_2 = 0$ were used by Gel'fand and Shapiro (Ref. 2) for solving the wave equation for the 3-vector potential in radiation gauge. The result, however, was not so simple as the one we obtain in this paper for Maxwell's fields. Reference to previous applications to solving the Dirac equation are also given in Ref. 2.

and, $\alpha^0_{\mp 1,0} \equiv 0$,

$$\alpha^j_{\mp 1,m} = \pm \frac{1}{[2j(j+1)]^{\frac{1}{2}}} \frac{1}{r}\left[\frac{\partial}{\partial r} \pm \frac{\partial}{\partial t}\right](r^2\alpha^j_{0,m}). \quad (5.4)$$

One can verify that a solution of Eq. (5.3) for α^j_{0m} along with $\alpha^j_{\pm 1,m}$ given by Eq. (5.4) indeed solves the original two equations, i.e., Eqs. (5.1) and (5.2). Equation (5.1) is trivially satisfied because of Eq. (5.4). Equation (5.2) is satisfied for any $\alpha^j_{\pm 1,m}$ satisfying Eq. (5.4) if α^j_{0m} satisfy Eq. (5.3). The case for which $j = 0$ needs special attention because of the presence of the factor $j(j+1)$ in Eqs. (5.1) and (5.2) which decouples the field functions. This case is discussed below.

We thus arrive at the conclusion that knowing $\alpha^j_{0,m}(t, r)$ leads to knowing $\alpha^j_{\pm 1,m}(t, r)$ completely. In other words, the most general solution of Maxwell's equations is effectively reduced to the solution of only one partial differential equation with two independent variables t and r.

The case of $j = 0$ (S wave) cannot be obtained as a particular case. From Eq. (5.1) we obtain ($m = 0$ also)

$$\left(\frac{\partial}{\partial r} \pm \frac{\partial}{\partial t}\right)[r^2\alpha^0_{00}(t, r)] = 0. \quad (5.5)$$

Accordingly, we have

$$\frac{\partial}{\partial r}(r^2\alpha^0_{00}) = \frac{\partial}{\partial t}(r^2\alpha^0_{00}) = 0. \quad (5.6)$$

The solution of this equation is

$$\alpha^0_{00} = Q/r^2, \quad (5.7)$$

where Q is a constant independent of t or r, and is, of course, the total charge of the system.

We now assume a solution of the form

$$\alpha^j_{0,m}(t, r) = r^{-2}\int R(k, r)e^{-ikt}\,dk \quad (5.8)$$

for Eq. (5.3). We obtain an ordinary differential equation for the new function $R(k, r)$:

$$\frac{d^2R}{dr^2} + \left[k^2 - \frac{j(j+1)}{r^2}\right]R = 0. \quad (5.9)$$

Equation (5.9) is the well-known partial-wave equation obtained from the Schrödinger equation for the zero-potential case. Its solutions are extensively discussed by de Alfaro and Regge.[13] The static case is particularly simple and is given below.

When we assume the solutions are time independent, Eq. (5.3) becomes

$$\frac{d^2}{dr^2}(r^2\alpha^j_{0,m}) - j(j+1)\alpha^j_{0,m} = 0, \quad (5.10)$$

where α^j_{0m} is now a function of r alone and α^0_{00} is given by Eq. (5.7). We notice that this equation is invariant under the change $j \to -(j+1)$. Therefore we try solutions of the form r^{j-1} and $r^{-(j+2)}$ to obtain

$$\alpha^j_{0,m}(r) = A^j_m jr^{j-1} + B^j_m(j+1)r^{-(j+2)}, \quad (5.11)$$

where A^j_m and B^j_m are constants (with $B^0_0 = Q$). The $\alpha^j_{\pm 1,m}(r)$ are then obtained from α^j_{0m} by Eq. (5.4):

$$\alpha^j_{\mp 1,m}(r) = \pm[\tfrac{1}{2}j(j+1)]^{\frac{1}{2}}[A^j_m r^{j-1} - B^j_m r^{-(j+2)}]. \quad (5.12)$$

The most general static solution of Maxwell's equations without sources is therefore given by

$$\eta_0(r, u) = \sum_{j=0}^{\infty}\sum_{n=-j}^{j}[A^j_n jr^{j-1} + B^j_n(j+1)r^{-(j+2)}]T^j_{0,n}(u), \quad (5.13)$$

$$\eta_{\pm}(r, u) = \mp\sum_{j=1}^{\infty}\sum_{n=-j}^{j}[\tfrac{1}{2}j(j+1)]^{\frac{1}{2}} \times [A^j_n r^{j-1} - B^j_n r^{-(j+2)}]T^j_{\pm 1,n}(u). \quad (5.14)$$

[13] V. de Alfaro and T. Regge, *Potential Scattering* (North-Holland Publ. Co., Amsterdam, 1965).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Generating Functions of Classical Groups and Evaluation of Partition Functions

T. S. SANTHANAM
MATSCIENCE, *The Institute of Mathematical Sciences, Madras, India*

(Received 14 July 1968)

The generating functions of classical groups are used to set up recursion relations for their partition functions. These are then used to find the internal multiplicity structure of the weights using Kostant's formula.

1. INTRODUCTION

The Clebsch–Gordan (CG) program of classical groups suffers from two major difficulties. Unlike the rotation group in three dimensions for which the CG program is well known, many other classical groups do not possess the properties of simple reducibility and the equivalence of an irreducible representation (IR) and its conjugate. Here by the lack of simple reducibility we mean the multiple occurrence of an IR in the product of two IR's. This multiplicity is called the external multiplicity.[1] However, many relations have been worked out[2,3] which relate this external multiplicity to the multiple occurrence of a given weight in an IR. This multiple occurrence of a given weight in an IR, a feature not shared by the IR's of $O(3)$, is called the internal (or inner) multiplicity structure.

At present the internal multiplicity structure can be worked out using Kostant's formula.[4] There exist, however, many other methods (for instance, the recursion method of Fraudenthal[5]), although in practice Kostant's formula is the most useful. Kostant's formula involves the partition function of expressing a nonnegative integral linear combination of positive roots in terms of a nonnegative integral linear combination of primitive roots. These partition functions have been known so far only for rank two and three groups.[6]

Recently we developed a method[7] of obtaining the partition functions for A_l ($\sim SU(l+1)$) by using the generating functions. In this, we set up recursion relations for the partition functions, which are then used in conjunction with Kostant's formula to compute the internal multiplicities. Of course, the calculation gets more and more involved as one goes to large l. However, the method is precise.

In this paper, we work out the generating functions for A_l, B_l, C_l, D_l, and G_2. The calculations for the other exceptional groups F_4, E_6, E_7, and E_8 will be published elsewhere. We also obtain recursion relations for the internal multiplicity.

In Sec. 2, the general discussion of Kostant's formula is given. We discuss the cases of $A_l \sim SU(l+1)$, $B_l \sim O(2l+1)$, $C_l \sim (Sp_{2l})$, $D_l \sim O(2l)$, and G_2 in Secs. 3 through 7. The discussion includes the Weyl group, the structure of positive and primitive (simple) roots and the Diophantine equations. Explicit formulas are obtained and possible recursion relations for the partition functions are given. In Sec. 8, the connection between internal and external multiplicity structures is discussed. In Sec. 9, the conclusions are given. Many of the properties of the classical groups (structure of positive and primitive roots and so on) are contained in many places. We have taken them from the papers of Dynkin.[8]

2. KOSTANT'S FORMULA

The inner multiplicity $M^m(m')$ of a weight m' belonging to the irreducible representation $D(m)$ of highest weight m is given by Kostant's formula,[4] which is

$$M^m(m') = \sum_{S \in W} \delta_S P[S(m + R_0) - (m' + R_0)], \quad (2.1)$$

where W is the Weyl group and R_0 is half the sum of positive roots. $\delta_S = \pm 1$ according as whether the reflection is even or odd, respectively. $P(M)$ is the partition function for the weight M. This is the number of ways the weight M can be written as a sum over all the positive roots

$$M = \sum_{i=1}^{n} a_i \varphi_i, \quad (2.2)$$

with different nonnegative integers a_i. On the other hand, Antoine and Speiser[9] have shown that the vector

$$S(m + R_0) - (m' + R_0)$$

[1] The terminology is from A. J. Macfarlane, L. O'Raifeartaigh, and P. S. Rao, J. Math. Phys. **8**, 536 (1967).
[2] L. C. Biedenharn, Phys. Letters **3**, 254 (1963); G. E. Baird and L. C. Biedenharn, J. Math. Phys. **5**, 1730 (1964).
[3] G. Racah, *Group Theoretical Concepts and Methods in Elementary Particle Physics*, F. Gürsey, Ed. (Gordon and Breach, Science Publishers, New York, 1964), p. 20; D. Speiser, *ibid.* p. 201.
[4] N. Jacobson, *Lie Algebras* (Interscience Publishers, Inc., New York, 1962), p. 261.
[5] Reference 4, p. 247.
[6] J. Tarski, J. Math. Phys. **4**, 569 (1963).
[7] T. S. Santhanam, MATSCIENCE Preprint MAT-3-1968.
[8] E. B. Dynkin, Am. Math. Soc. Transl. (2) **6**, 353 (1957).
[9] J. P. Antoine and D. Speiser, J. Math. Phys. **5**, 1226, 1560 (1964).

can be expressed for a fixed $S \in W$ uniquely in terms of the primitive roots as

$$S(m + R_0) - (m' + R_0) = \sum_{i=1}^{l} k_i B_i, \qquad (2.3)$$

l being the rank of the group. From (2.2) and (2.3), it is clear that $P(M)$ is the number of ways we can write

$$\sum_{i=1}^{l} k_i B_i = \sum_{\mu=1}^{n} a_\mu \varphi_\mu, \quad k_i \geq 0, \quad a_\mu \geq 0, \qquad (2.4)$$

where k_i and a_μ are integers for given k_i. It can be shown that $P(k_1, \cdots, k_l)$ is the multiplicity $\bar{M}(\gamma)$ of a vector γ of $1/\Delta$ (Ref. 9), where the $1/\Delta$ is related to the character by Weyl's formula

$$\chi^m(\xi) = [x(m + R_0)]/\Delta, \quad \Delta = x(R_0). \qquad (2.5)$$

$x(m + R_0)$ is the alternating elementary sum, such that

$$x(m + R_0) = \sum_{S \in W} \delta_S \exp i[S(m + R_0), \xi], \qquad (2.6)$$

and $[S(m + R_0), \xi]$ denotes the Cartan-Killing form of the scalar product where the ξ are the coordinates of the toroid (the group parameters). Hence (2.1) can be written as

$$M^m(m') = \sum_{S \in W} \delta_S \bar{M}(k_1^S, k_2^S, \cdots, k_l^S).$$

If we can calculate the partition function $\bar{M}(k_1^S, \cdots, k_l^S)$, then $M^m(m')$ can be computed in principle. In the following few sections, we explicitly calculate $\bar{M}(k_1^S, \cdots, k_l^S)$ for the various classical groups.

3. A_l ($\sim SU(l + 1)$)

The roots of this algebra are given by $e_i - e_j$, $i, j = 1, \cdots, (l + 1)$. The e_i form an orthogonal basis in $(l + 1)$-dimensional space in which the roots and weights are defined. There are $l(l + 1)$ roots. The $\frac{1}{2}l(l + 1)$ positive roots are then obtained as $e_i - e_j$ $(i < j)$. The primitive (simple) roots in this case are $B_i = e_i - e_{i+1}$, $i = 1, 2, \cdots, l$. Equation (2.4) then can be written as

$$K_i = C_{i\mu} a_\mu, \quad i = 1, \cdots, l, \quad \mu = 1, \cdots, \tfrac{1}{2}l(l + 1), \qquad (3.1)$$

where C is the $[\frac{1}{2}l(l + 1) \times l]$-dimensional rectangular matrix

$$C_{i\mu} = \begin{array}{c} \\ i = 1, \cdots, l \downarrow \end{array} \overset{\rightarrow \mu = 1, \cdots, \frac{1}{2}l(l+1)}{\left(\begin{array}{cccc|cccc|ccccc|c} 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & \cdots & 1 \\ 0 & 1 & \cdots & 0 & 1 & 1 & \cdots & 0 & 1 & 1 & \cdots & 0 & \cdots & 1 \\ 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 & 1 & 1 & \cdots & 0 & \cdots & 1 \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 & \cdots & 1 \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 1 \\ \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & & \cdot \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1 & \cdots & 1 \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 1 & \cdots & 1 \\ 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 1 & \cdots & 1 \end{array}\right)} \qquad (3.2)$$

It can easily be seen that only for the case of $l = 1$, the matrix C is a nonsingular square matrix (a number) so that there is a unique solution, i.e., $\bar{M}(k_1) = 1$. However, in general, C is a rectangular matrix and so, given the vector k and the matrix C, the number of a's is trivially infinite, and it is only because we have the restriction that the elements of the matrix C are nonnegative integers that the very question of the number of solutions (number of a's, the components of the vector a are again nonnegative integers) makes a meaning after all. We recognize that the number of solutions of Eq. (2.4) is given by the coefficient of $x_1^{k_1} x_2^{k_2} \cdots x_l^{k_l}$ of the generating functions. To solve the Diophantine equations (3.1) (actually, we mean finding the number of solutions for given k and C), we now use the method of generating functions.[7] Let $f(x_1, \cdots, x_l)$ be the generating function, defined by

$$f_l(x_1, \cdots, x_l) = \prod_{i=1}^{\frac{1}{2}l(l+1)} \frac{1}{(1 - x_1^{C_{1i}} x_2^{C_{2i}} \cdots x_l^{C_{li}})}, \qquad (3.3)$$

where $x_1, \cdots, x_l$ are chosen arbitrary parameters with modulus less than one. $\bar{M}(k_1, \cdots, k_l)$ is now given by the coefficient of $x_1^{k_1} x_2^{k_2} \cdots x_l^{k_l}$ in $f_l(x_1, \cdots, x_l)$. This can be checked by actually expanding f_l

in power series. Since the matrix C is known, we can write the following important relation:

$$f_l(x_1, \cdots, x_l) = \left[\prod_{i=1}^{l}\left(1 - \prod_{j=l-i+1}^{l} x_j\right)\right]^{-1} f_{l-1}(x_1, \cdots, x_{l-1}). \quad (3.4)$$

Now, we can expand (3.4) in power series. $\bar{M}(k_1, \cdots, k_l)$ is the coefficient of $x_1^{k_1}x_2^{k_2}\cdots x_l^{k_l}$ in (3.4). If $\bar{M}(k_1, \cdots, k_{l-1})$ is the coefficient of $x_1^{k_1}x_2^{k_2}\cdots x_{l-1}^{k_{l-1}}$ in $f_{l-1}(x_1, \cdots, x_{l-1})$, then it is easily seen that

$$\bar{M}(k_1, \cdots, k_l) = \sum_{r_{l-1}=0}^{\infty}\cdots\sum_{r_2=0}^{\infty}\sum_{r_1=0}^{\infty}\bar{M}(k_1 - r_1; k_2 - r_1 - r_2; \cdots; k_{l-1} - r_1 - r_2 - \cdots - r_{l-1}) \quad (3.5)$$

with

$$0 \le r_1 \le k_1; 0 \le r_1 + r_2 \le k_2; \cdots;$$
$$0 \le r_1 + r_2 + \cdots + r_{l-1} \le k_{l-1},$$

and

$$r_1 + r_2 + \cdots + r_l = k_l,$$

so that

$$0 \le r_1 + r_2 + \cdots + r_{l-1} \le \min(k_l, k_{l-1}).$$

Define a new set of variables as follows:

$$i_1 = r_1; i_2 = r_1 + r_2; \cdots;$$
$$i_{l-1} = r_1 + r_2 + \cdots + r_{l-1}; \quad (3.6)$$

then

$$\bar{M}(k_1, \cdots, k_l) = \sum_{i_{l-1}=i_{l-2}}^{\min(k_{l-1},k_l)}\sum_{i_{l-2}=i_{l-3}}^{k_{l-2}}\cdots\sum_{i_2=i_1}^{k_2}\sum_{i_1=0}^{k_1} \times \bar{M}(k_1 - i_1; k_2 - i_2; \cdots; k_{l-1} - i_{l-1}). \quad (3.7)$$

Equation (3.7) is exactly the recursion relation we want, since it facilitates the computation of the partition function for any A_l (l arbitrary) in terms of the simple partition function for A_2, viz.,

$$\bar{M}(k_1, k_2) = \sum_{0}^{\min(k_1,k_2)} 1 = 1 + \min(k_1, k_2), \quad (3.8)$$

which has been obtained earlier.[10] The weight space is again $(l+1)$-dimensional with the condition on the components of a weight m that

$$\sum_{i=1}^{l+1} m_i = 0.$$

Using Weyl's theorems, it can be proved that the components are (integer)/$(l+1)$. The Weyl group in this case permutes the components of m and is of order $(l+1)!$ The dominant weights satisfy

$$m_1 \ge m_2 \ge \cdots \ge m_{l+1}, \quad \sum_{i=1}^{l+1} m_i = 0. \quad (3.9)$$

These properties of the dominant weight are used in picking up the nonvanishing contributions to $M^m(m')$.

4. B_l ($\sim O_{2l+1}$)

The roots of this algebra are $\pm(e_i \pm e_j)$, $\pm e_i$ $(i = 1, \cdots, l)$. There are $2l^2$ of them. The l^2 positive roots may be obtained as $e_i - e_j$, $e_i + e_j$, and e_i $(i < j)$. The simple roots in this case are given by $B_{i-1} = e_{i-1} - e_i$, $B_l = e_l$. Equation (2.4) then takes the form

$$K_i = C_{i\mu}a_\mu, \quad i = 1, \cdots, l, \quad \mu = 1, \cdots, l^2, \quad (4.1)$$

where C is the $(l^2 \times l)$-dimensional rectangular matrix

$$C_{i\mu} = \left(\begin{array}{c} \\ i = 1, \cdots, l \\ \downarrow \end{array}\right. \overset{C^{A_l}}{\underset{\frac{1}{2}l(l+1)}{\longleftarrow}} \left.\begin{array}{c} \\ \\ \end{array}\right) \begin{array}{c} \\ \rightarrow \mu = 1, \cdots, l^2 \end{array}$$

$$\left(\begin{array}{cccc|cccc|c} 1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 & \cdots \\ 1 & 1 & \cdots & 2 & 1 & 1 & \cdots & 1 & \cdots \\ 1 & 1 & \cdots & 2 & 1 & 1 & \cdots & 2 & \cdots \\ \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & \\ \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & \\ \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & \\ 1 & 1 & \cdots & 2 & 1 & 1 & \cdots & 2 & \cdots \\ 1 & 2 & \cdots & 2 & 1 & 2 & \cdots & 2 & \cdots \\ 2 & 2 & \cdots & 2 & 2 & 2 & \cdots & 2 & \cdots \end{array}\right. \begin{array}{c} 0 \\ 0 \\ 0 \\ \\ \\ \\ 0 \\ 1 \\ 2 \end{array}\left.\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \end{array}\right) \quad (4.2)$$

The generating function in this case is

$$f_l^{B_l}(x_1, \cdots, x_l) = \prod_{i=1}^{l^2}\frac{1}{(1 - x_1^{C_{1i}}x_2^{C_{2i}}\cdots x_l^{C_{li}})}. \quad (4.3)$$

It can be easily checked that, unlike the case of A_l, there is no simple recursion relation between $f_l^{B_l}$ and $f_{l-1}^{B_{l-1}}$. However, the following very interesting relation can be obtained, which of course is obvious from

[10] B. Gruber and T. S. Santhanam, Nuovo Cimento **45A**, 1046 (1966).

the structure of the C matrix, Eq. (4.2):

$$f_l^{B_l}(x_1, \cdots, x_l) = \frac{f_l^{A_l}(x_1, \cdots, x_l)}{\prod_{i=2}^{l} \prod_{j=0}^{l-i} \left(1 - \prod_{K=i-1}^{l} x_K \prod_{r=l-j}^{l} x_r\right)} \tag{4.4}$$

It is, therefore, clear that for large values of l the recursion relation, Eq. (4.4), is not simple. For $l = 2$, Eq. (4.4) reads as

$$f_2^{B_2}(x_1, x_2) = \frac{f_2^{A_2}(x_1, x_2)}{(1 - x_1 x_2^2)}, \tag{4.5}$$

so that the recursion relation for $\bar{M}$ is

$$\bar{M}^{B_2}(k_1, k_2) = \sum_i \bar{M}^{A_2}(k_1 - i; k_2 - 2i), \tag{4.6}$$

which is the relation obtained by Gruber and Zaccaria earlier.[11]

The weight space is l-dimensional and the components may be integers or half-integers. The Weyl group in this case consists of all possible permutations of the components of m together with all possible changes of sign and is therefore of order $2^l l!$. The dominant weights satisfy

$$m_1 \geq m_2 \geq \cdots \geq m_l \geq 0. \tag{4.7}$$

5. C_l ($\sim Sp(2l)$)

The roots of this algebra are $\pm(e_i \pm e_j)$, $\pm 2e_i$ $(i = 1, \cdots, l)$. It should be stressed that the factor 2 in the second class of roots is very important and makes this algebra different from B_l. There are $2l^2$ roots. The l^2 positive roots are given by $e_i - e_j$, $e_i + e_j$, $2e_i$ $(i < j)$. The simple roots in this case are $B_{i-1} = e_{i-1} - e_i$ $(i = 1, \cdots, l)$, $B_l = 2e_l$. Equation (2.4) is then

$$\begin{aligned} K_i &= C_{i\mu} a_\mu, \\ i &= 1, \cdots, l, \\ \mu &= 1, \cdots, l^2, \end{aligned} \tag{5.1}$$

where C is the $(l^2 \times l)$-dimensional rectangular matrix

$$C_{i\mu} = \left(\begin{array}{c} i = 1, \cdots, l \downarrow \end{array} \right. \quad \overset{C^{A_l}}{\underset{\frac{1}{2}l(l+1)}{\longleftrightarrow}} \quad \left| \begin{array}{cccc|ccc|c} 1 & 1 & \cdots & 2 & 0 & \cdots & 0 & \cdots \\ 1 & 1 & \cdots & 2 & 1 & \cdots & 2 & \cdots \\ 1 & 1 & \cdots & 2 & 1 & \cdots & 2 & \cdots \\ \cdot & \cdot & & \cdot & \cdot & & \cdot & \\ \cdot & \cdot & & \cdot & \cdot & & \cdot & \\ \cdot & \cdot & & \cdot & \cdot & & \cdot & \\ 1 & 2 & \cdots & 2 & 1 & \cdots & 2 & \cdots \\ 2 & 2 & \cdots & 2 & 2 & \cdots & 2 & \cdots \\ 1 & 1 & \cdots & 1 & 1 & \cdots & 1 & \cdots \end{array} \right. \quad \left. \begin{array}{c} 0 \\ 0 \\ 0 \\ \\ \\ \\ 0 \\ 2 \\ 1 \end{array} \right) \quad \rightarrow \mu = 1, \cdots, l^2 \tag{5.2}$$

The generating function is of the same type of $f_l^{B_l}(x_1, \cdots, x_l)$, but the elements of C are different in view of Eq. (5.2). Again in this case, there is no simple recursion relation between $f_l^{C_l}$ and $f_{l-1}^{C_{l-1}}$. However, the following relation can be easily verified:

$$f_l^{C_l}(x_1, \cdots, x_l) = \frac{f_l^{A_l}(x_1, \cdots, x_l)}{\prod_{i=1}^{l} \prod_{j=1}^{l-i} \left(1 - \prod_{K=i}^{l} x_K \prod_{r=l-j}^{l-1} x_r\right)}. \tag{5.3}$$

For the special case of $l = 2$, the above relation reads as

$$f_2^{C_2}(x_1, x_2) = \frac{f_2^{A_2}(x_1, x_2)}{(1 - x_1^2 x_2)}, \tag{5.4}$$

so that the same relation (4.6) is derived with $k_1 \leftrightarrow k_2$ as

$$\bar{M}^{C_2}(k_1, k_2) = \sum_i \bar{M}(k_1 - 2i; k_2 - i). \tag{5.5}$$

This is not surprising because of the known isomorphism between C_2 and B_2.

The weight space is again l-dimensional and the components of the weight are integers. The Weyl group is the same as that for B_l and is of order $2^l l!$. This consists of all the permutations of the components of the weight and all changes in sign. The dominant weight satisfies

$$m_1 \geq m_2 \geq \cdots \geq m_l \geq 0. \tag{5.6}$$

6. D_l ($\sim O(2l)$)

The roots are given by $\pm(e_i \pm e_j)$, $i, j = 1, \cdots, l$, and there are $2(l^2 - l)$ of them. The $l(l-1)$ positive roots are then $e_i + e_j$ and $e_i - e_j$ $(i < j)$. The simple roots are $B_{i-1} = e_{i-1} - e_i$ and $B_l = e_{l-1} + e_l$. Equation (2.4) is then

$$\begin{aligned} K_i &= C_{i\mu} a_\mu, \\ i &= 1, \cdots, l, \\ \mu &= 1, \cdots, l(l-1), \end{aligned} \tag{6.1}$$

[11] B. Gruber and F. Zaccaria, Nuovo Cimento Suppl. 5, 914 (1967).

where C is the $[l(l-1) \times l]$-dimensional rectangular matrix

$$C_{i\mu} = \begin{matrix} \\ i = 1, \cdots, l \downarrow \end{matrix} \begin{matrix} \\ \xleftarrow[\frac{1}{2}l(l+1)-1]{C^{A_l'}} \end{matrix} \begin{matrix} \rightarrow \mu = 1, \cdots, l(l-1) \\ \left(\begin{array}{c|ccc|ccc|ccc|c} 1 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1 & 0 & \cdots & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 0 & 1 & 1 & \cdots & 2 & 1 & \cdots & 1 & \cdots & 0 \\ 1 & 1 & \cdots & 0 & 1 & 1 & \cdots & 2 & 1 & \cdots & 2 & \cdots & 0 \\ \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & \cdot & & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & \cdot & & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & \cdot & & \cdot & \cdot & & \cdot & & \cdot \\ 1 & 1 & \cdots & 0 & 1 & 2 & \cdots & 2 & 1 & \cdots & 2 & \cdots & 1 \\ 1 & 1 & \cdots & 1 & 2 & 2 & \cdots & 2 & 2 & \cdots & 2 & \cdots & 2 \\ 0 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1 & 1 & \cdots & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 & 1 & 1 & \cdots & 1 & 1 & \cdots & 1 & \cdots & 1 \end{array} \right) \end{matrix}, \tag{6.2}$$

where $C^{A_l'}$ denotes the matrix C^{A_l} with the column $(0, 0, \cdots, 0, 1, 1)$ missing. In this case also, there is the following recursion relation:

$$f_l^{D_l}(x_1, \cdots, x_l) = \frac{f_l^{A_l}(x_1, \cdots, x_l)[1 - x_{l-1}x_l]}{\left[\prod_{K=2}^{l-2}\left(1 - \prod_{r=l-K}^{l-2} x_r x_l\right)\right]\left[\prod_{r=0}^{l-4}\prod_{K=0}^{l-r-4}\left(1 - \prod_{s=r+1}^{l} x_s \prod_{t=l-K-2-r}^{l-2} x_t\right)\right]}. \tag{6.3}$$

For $l = 2$, the above relation gives

$$\begin{aligned} f_2^{D_2}(x_1, x_2) &= f_2^{A_2}(x_1, x_2)(1 - x_1x_2) \\ &= [(1 - x_1)(1 - x_2)]^{-1}, \end{aligned} \tag{6.4}$$

and so $\bar{M}(k_1, k_2) = 1$ for all k_1, k_2. This, of course, is a known result. For $l = 3$, this yields

$$f_3^{D_3}(x_1, x_2, x_3) = \frac{f_3^{A_3}(x_1, x_2, x_3)(1 - x_2x_3)}{(1 - x_1x_3)}, \tag{6.5}$$

so that

$$\begin{aligned} &\bar{M}(k_1, k_2, k_3) \\ &\quad = \sum_{i=0}^{\min(k_1, k_3)} \bar{M}^{A_3}(k_1 - i; k_2; k_3 - i) \\ &\qquad - \sum_{i=0}^{\min(k_1, k_3-1)} \bar{M}^{A_3}(k_1 - i; k_2 - 1; k_3 - i - 1). \end{aligned} \tag{6.6}$$

The weight space is l-dimensional. The components of the weight must be integers or half-integers. The Weyl group in this case consists of all permutations of the components of the weight (corresponding to the reflection perpendicular to the roots $e_i - e_j$) and all changes of sign *in pairs* (corresponding to the reflection perpendicular to the roots $e_i + e_j$) and is of order $2^{l-1}l!$.

The condition for a weight to be dominant is

$$m_1 \geq m_2 \geq \cdots \geq m_{l-1} \geq |m_l|.$$

7. G_2

The roots for this exceptional group are $\pm(e_i - e_j)$, $\pm e_i$, $i, j = 1, 2, 3$; $e_3 = -(e_1 + e_2)$. The six positive roots are $(e_1 - e_2)$, $(e_1 - e_3)$, $(e_2 - e_3)$, e_1, e_2, and $-e_3 = (e_1 + e_2)$. The simple roots are $B_1 = e_1 - e_2$ and $B_2 = e_2$. Equation (2.4) then becomes

$$\begin{aligned} K_i &= C_{i\mu}a_\mu, \\ i &= 1, 2, \\ \mu &= 1, 2, \cdots, 6, \end{aligned} \tag{7.1}$$

where the (6×2) rectangular matrix C is

$$C_{i\mu} = \begin{matrix} \\ i = 1, 2 \downarrow \end{matrix} \begin{matrix} \mu = 1, \cdots, 6 \\ \begin{pmatrix} 1 & 0 & 1 & 1 & 1 & 2 \\ 0 & 1 & 1 & 2 & 3 & 3 \end{pmatrix} \end{matrix}. \tag{7.2}$$

The generating function is then

$$\begin{aligned} &f^{G_2}(x_1, x_2) \\ &\quad = (1 - x_1)^{-1}(1 - x_2)^{-1}(1 - x_1x_2)^{-1} \\ &\qquad \times (1 - x_1x_2^2)^{-1}(1 - x_1x_2^3)^{-1}(1 - x_1^2x_2^3)^{-1}, \end{aligned} \tag{7.3}$$

and so one immediately sees the following relations:

$$\begin{aligned} f^{G_2}(x_1, x_2) &= \frac{f_2^{A_2}(x_1, x_2)}{(1 - x_1x_2^2)(1 - x_1x_2^3)(1 - x_1^2x_2^3)} \\ &= \frac{f_2^{B_2}(x_1, x_2)}{(1 - x_1x_2^3)(1 - x_1^2x_2^3)}. \end{aligned} \tag{7.4}$$

It follows, therefore,[11,12] that

$$\begin{aligned} &\bar{M}^{G_2}(k_1, k_2) \\ &\quad = \sum_{i,j,k} \bar{M}^{A_2}(k_1 - i - j - 2k; k_2 - 2i - 3j - 3k). \end{aligned} \tag{7.5}$$

[12] D. Radhakrishnan and T. S. Santhanam, J. Math. Phys. **8**, 2206 (1967).

The above sum has been explicitly carried out in Ref. 12 for various inequalities of k_1 and k_2. From (7.4) it also follows that

$$\bar{M}^{G_2}(k_1, k_2) = \sum_{i,j} \bar{M}^{B_2}(k_1 - i - 2j; k_2 - 3i - 3j). \quad (7.6)$$

The weight space in this case is again three-dimensional like A_2 with the components of a weight satisfying

$$m_1 + m_2 + m_3 = 0.$$

The components of the weights are integers. The Weyl group is of order 12 and consists of the six permutations of (m_1, m_2, m_3) corresponding to the reflection perpendicular to the roots $(e_1 - e_2)$, $(e_2 - e_3)$, $(e_1 - e_3)$, and six permutations with a total change in sign corresponding to the roots e_i. The dominant weight satisfies

$$m_1 \geq m_2 \geq m_3; \quad m_1 \geq 0, \quad m_2 \leq 0, \quad m_3 \leq 0. \quad (7.7)$$

8. EXTERNAL MULTIPLICITY

In the case of rotation groups in three dimensions, an IR is characterized by the eigenvalue j of the single Casimir operator J^2, which is integral or half-integral. One is then familiar with the CG series

$$D^{j_1} \otimes D^{j_2} = \sum_{j=j_1+j_2}^{|j_1-j_2|} \otimes D^j, \quad (8.1)$$

where D^j denotes an IR with the highest weight j. If $j_1 > j_2$ (in which case we say that the representation D^{j_1} dominates D^{j_2}), the right-hand side of (8.1) can be interpreted as those IR's whose highest weights are obtained by adding to the highest weight of the dominant IR, i.e., D^{j_1}, all the weights of the IR D^{j_2} (from j_2 to $-j_2$). This is the main constant of Biedenharn's theorem.[2] The condition for one IR to dominate another IR have been worked out.[1] The general idea follows from the two equivalent formulas for the character

$$\chi^m(\xi) = \sum_{m' \in D(m)} M^m(m') \exp i(m', \xi), \quad (8.2)$$

where the $\chi^m(\xi)$ is the character of an IR with the highest weight m and ξ are the group parameters. The other formula is

$$\chi^m(\xi) = \frac{x(m + R_0)}{x(R_0)}, \quad (8.3)$$

where

$$x(m + R_0) = \sum_{S \in W} \delta_S \exp i[S(m + R_0), \xi].$$

Suppose that we are interested in the product of IR's $D(\Lambda_1)$ and $D(\Lambda_2)$ with Λ_1 and Λ_2 as their highest weights, respectively. Then

$$\chi(\Lambda_1)\chi(\Lambda_2) = \frac{\sum_{S \in W} \delta_S \exp i[S(\Lambda_1 + R_0), \xi]}{\sum_{S \in W} \delta_S \exp i[S(R_0), \xi]} \times \sum_{m' \in D(\Lambda_2)} M^{\Lambda_2}(m') \exp i(m', \xi), \quad (8.4)$$

where we have used Eq. (8.2) for $\chi(\Lambda_2)$ and (8.3) for $\chi(\Lambda_1)$. Equation (8.4) can now be regrouped to be written as

$$\chi(\Lambda_1)\chi(\Lambda_2) = \frac{\sum_{S \in W} \sum_{m' \in D(\Lambda_2)} \delta_S M^{\Lambda_2}(m') \exp i[S(\Lambda_1 + m' + R_0), \xi]}{\sum_{S \in W} \delta_S \exp i[S(R_0), \xi]}, \quad (8.5)$$

where we have used the property

$$S(P) + S(Q) = S(P + Q). \quad (8.6)$$

Equation (8.5) can now be interpreted as follows. In the product $D(\Lambda_1) \otimes D(\Lambda_2)$, where $D(\Lambda_1)$ dominates $D(\Lambda_2)$, only those IR's with the highest weight $(\Lambda_1 + m')$, $m' \in D(\Lambda_2)$, occur in the reduction. These IR's occur with the multiplicity $M^{\Lambda_2}(m')$, i.e., multiplicity of the weight m' in the IR with highest weight Λ_2. The condition of dominance of one IR over the other is needed to make the $(\Lambda_1 + m')$ dominant. These have been the more general formulas of Racah and Speiser[3] which do not involve the condition that one IR dominate the other. For our purpose, Eq. (8.5) is quite sufficient. Thus, we realize that the external multiplicity is very closely related to the internal multiplicity structure.

9. CONCLUSION

We have constructed generating functions for the various classical groups. A_l, B_l, C_l, D_l, and G_2. These are then used to set up recursion relations for the partition function which enter Kostant's formula for the inner multiplicity structure. The essential idea of the whole analysis is the realization that the number of solutions of the matrix equation $K = Ca$ (for given k and c), where the matrix C is in general a rectangular matrix with nonnegative-integer coefficients and the components of the vectors k and a are again nonnegative integers, is given by the coefficient of $x_1^{k_1} \cdots x_l^{k_l}$ of the generating function. In many cases, the explicit evaluation of the number of solutions is not possible, and so we have set up recursion relations. While in the case of A_l the recursion relation is between the partition functions

of A_l and A_{l-1}, in the cases of B_l, C_l, and D_l the recursion relations for their functions are among these and of A_l. For $G(2)$, there are two recursion relations, one with A_2 and the other with B_2. We have also discussed the connection between the internal and external multiplicity structures.

ACKNOWLEDGMENTS

It is a pleasure to thank Professor Alladi Ramakrishnan for encouragement and very useful discussions on the matrix problem discussed in the text. The various fruitful discussions with the academic group of the Institute are gratefully acknowledged.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Representation Theory of $SP(4)$ and $SO(5)$*

WAYNE J. HOLMAN, III
Center for Theoretical Studies, University of Miami, Coral Gables, Florida

(Received 3 May 1968)

The basis states for all the irreducible unitary representations of $Sp(4)$ are constructed by means of a calculus of boson operators. The Gel'fand states are explicitly expanded in terms of their constituent Weyl patterns. In terms of these states the matrix elements of finite rotations in five dimensions are obtained.

1. INTRODUCTION

The locally isomorphic groups $Sp(4)$ and $SO(5)$ have become of interest in physics from the two different standpoints of collective excitations of nuclei and space–time symmetries. The collective states of certain even–even nuclei have been represented by means of a five-dimensional isotropic harmonic oscillator which describes the quadrupole vibrations of the nuclear surface about a spherical equilibrium shape.[1–5] The predictions of this model have not all been observed to hold in actual nuclei, but it has, none the less, proved to be a convenient starting point for the description of that coupling of collective modes to the giant dipole oscillations which results in the splitting of the giant dipole resonance.[6,7] For the five-dimensional oscillator, which has the symmetry group $SU(5)$, only the totally symmetric irreducible representations of $SU(5)$ occur, and these may be considered to be fully reduced with respect to the $SO(5)$ subgroup.

In addition, Flowers[8] has achieved a classification of shell-model states and the group-theoretical definition of "seniority" in j–j coupling in terms of the symplectic group in $4j + 2$ dimensions. Helmers[9] subsequently studied the relation between these classifications for various nucleon numbers and found that it was governed by a different symplectic group, the transformations of which change the nucleon number. He found that the ten invariants, bilinear in the fermion operators, which commute with the operators of the symplectic group in $4j + 2$ dimensions, form the infinitesimal operators which generate a group with the structure of $SO(5) \simeq Sp(4)$.

This group is also of interest from the standpoint of space–time symmetries. The irreducible unitary representation functions of $SO(5)$ can be continued analytically to those of the de Sitter groups $SO(4, 1)$ and $SO(3, 2)$, whose contraction in the sense of Wigner and Inönü to the representations of the Poincaré group have been discussed by a number of authors,[10,11] especially by Ström,[10] who has obtained

* This work was supported by National Aeronautics and Space Administration Contract No. NASA NGR 10-007-010 and by Air Force Office of Scientific Research Contract No. AF AFOSR 1268-67.

[1] A. Bohr, Kgl. Danske Videnskab. Selskab, Met.-Fys. Medd. **26**, No. 14 (1952); A. Bohr and B. R. Mottelson, Kgl. Danske Videnskab. Selskab, Met.-Fys. Medd. **27**, No. 16 (1953).

[2] D. C. Choudhuri, Kgl. Danske Videnskab. Selskab, Met.-Fys. Medd. **28**, No. 4 (1954).

[3] K. W. Ford and C. A. Levinson, Phys. Rev. **100**, 1 (1955).

[4] B. J. Raz, Phys. Rev. **114**, 1116 (1959).

[5] B. F. Bayman and L. Silverberg, Nucl. Phys. **16**, 625 (1960).

[6] J. Le Tourneux, Kgl. Danske Videnskab. Selskab, Met.-Fys. Medd. **34**, No. 11 (1965).

[7] M. G. Huber, H. J. Weber, and W. Greiner (to be published).

[8] B. H. Flowers, Proc. Roy. Soc. (London) **A212**, 248 (1952).

[9] K. Helmers, Nucl. Phys. **23**, 594 (1961).

[10] S. Ström, Arkiv Fysik **30**, 455 (1965).

[11] N. T. Evans, J. Math. Phys. **8**, 170 (1967).

of A_l and A_{l-1}, in the cases of B_l, C_l, and D_l the recursion relations for their functions are among these and of A_l. For $G(2)$, there are two recursion relations, one with A_2 and the other with B_2. We have also discussed the connection between the internal and external multiplicity structures.

ACKNOWLEDGMENTS

It is a pleasure to thank Professor Alladi Ramakrishnan for encouragement and very useful discussions on the matrix problem discussed in the text. The various fruitful discussions with the academic group of the Institute are gratefully acknowledged.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Representation Theory of $SP(4)$ and $SO(5)$*

WAYNE J. HOLMAN, III
Center for Theoretical Studies, University of Miami, Coral Gables, Florida

(Received 3 May 1968)

The basis states for all the irreducible unitary representations of $Sp(4)$ are constructed by means of a calculus of boson operators. The Gel'fand states are explicitly expanded in terms of their constituent Weyl patterns. In terms of these states the matrix elements of finite rotations in five dimensions are obtained.

1. INTRODUCTION

The locally isomorphic groups $Sp(4)$ and $SO(5)$ have become of interest in physics from the two different standpoints of collective excitations of nuclei and space–time symmetries. The collective states of certain even–even nuclei have been represented by means of a five-dimensional isotropic harmonic oscillator which describes the quadrupole vibrations of the nuclear surface about a spherical equilibrium shape.[1–5] The predictions of this model have not all been observed to hold in actual nuclei, but it has, none the less, proved to be a convenient starting point for the description of that coupling of collective modes to the giant dipole oscillations which results in the splitting of the giant dipole resonance.[6,7] For the five-dimensional oscillator, which has the symmetry group $SU(5)$, only the totally symmetric irreducible representations of $SU(5)$ occur, and these may be considered to be fully reduced with respect to the $SO(5)$ subgroup.

In addition, Flowers[8] has achieved a classification of shell-model states and the group-theoretical definition of "seniority" in j–j coupling in terms of the symplectic group in $4j + 2$ dimensions. Helmers[9] subsequently studied the relation between these classifications for various nucleon numbers and found that it was governed by a different symplectic group, the transformations of which change the nucleon number. He found that the ten invariants, bilinear in the fermion operators, which commute with the operators of the symplectic group in $4j + 2$ dimensions, form the infinitesimal operators which generate a group with the structure of $SO(5) \simeq Sp(4)$.

This group is also of interest from the standpoint of space–time symmetries. The irreducible unitary representation functions of $SO(5)$ can be continued analytically to those of the de Sitter groups $SO(4, 1)$ and $SO(3, 2)$, whose contraction in the sense of Wigner and Inönü to the representations of the Poincaré group have been discussed by a number of authors,[10,11] especially by Ström,[10] who has obtained

* This work was supported by National Aeronautics and Space Administration Contract No. NASA NGR 10-007-010 and by Air Force Office of Scientific Research Contract No. AF AFOSR 1268-67.

[1] A. Bohr, Kgl. Danske Videnskab. Selskab, Met.-Fys. Medd. **26**, No. 14 (1952); A. Bohr and B. R. Mottelson, Kgl. Danske Videnskab. Selskab, Met.-Fys. Medd. **27**, No. 16 (1953).

[2] D. C. Choudhuri, Kgl. Danske Videnskab. Selskab, Met.-Fys. Medd. **28**, No. 4 (1954).

[3] K. W. Ford and C. A. Levinson, Phys. Rev. **100**, 1 (1955).

[4] B. J. Raz, Phys. Rev. **114**, 1116 (1959).

[5] B. F. Bayman and L. Silverberg, Nucl. Phys. **16**, 625 (1960).

[6] J. Le Tourneux, Kgl. Danske Videnskab. Selskab, Met.-Fys. Medd. **34**, No. 11 (1965).

[7] M. G. Huber, H. J. Weber, and W. Greiner (to be published).

[8] B. H. Flowers, Proc. Roy. Soc. (London) **A212**, 248 (1952).

[9] K. Helmers, Nucl. Phys. **23**, 594 (1961).

[10] S. Ström, Arkiv Fysik **30**, 455 (1965).

[11] N. T. Evans, J. Math. Phys. **8**, 170 (1967).

the contraction of the basis states of the $SO(4, 1)$ representations to those of the Poincaré group, the latter being reduced in a helicity angular-momentum basis. The representations of the group in this basis have been discussed by Lomont and Moses,[12,13] who did not obtain them in global form.

From the purely mathematical standpoint, the representation theory of $Sp(4)$ and $SO(5)$ is interesting because it is the classical group of lowest parameter which exhibits the peculiar structural properties of the symplectic and orthogonal groups as they differ from those of the unitary groups. The classification program of the irreducible representations of the latter groups is based on the facts that (1) all irreducible representations of $U(n)$ can be projected out of tensor products of the defining n-dimensional representation; and (2) the transformation of the carrier space $A_{i_1}A_{i_2}\cdots A_{i_p} = B$, where each A denotes an n-dimensional vector space, by the tensor product of p of the defining representations commutes with all of the permutations of the p indices $i_1, \cdots, i_p$, i.e., with the elements of the symmetric group $S(p)$ operating on those indices.[14,15] Each of the irreducible representations of $S(p)$ is described by its Young symmetry pattern, defined by the partitions of p, and each pattern denotes uniquely an irreducible subspace of B. The Young symmetrizer, then, which projects the direct product space into the invariant subspace defined by the Young symmetry pattern, commutes with the tensor product of p of the defining representations of $U(n)$, and so reduces this tensor product into irreducible representations.

For the orthogonal groups the operation of taking the trace of any two indices of the carrier space also commutes with its transformation by the tensor product of p of the defining representations. This fact has the consequence that the carrier space of the representations of $O(n)$ is just the space of all traceless tensors, i.e., of those tensors each of whose traces is zero. It has the further consequence that irreducible representations of the orthogonal groups have only those Young patterns which have a total number of nodes in the first two columns less than or equal to n.

For the symplectic groups $Sp(n)$ the operation of taking the symplectic trace on any two indices of the carrier space commutes with transformation by the tensor product of defining representations; we have from this fact the consequence that the carrier space of the irreducible representations is the subspace of B, all of whose symplectic traces are zero, and ultimately that the irreducible representations of $Sp(n)$ have Young diagrams with no more than $\frac{1}{2}n$ rows.

The consequences of these additional algebraic conditions on the carrier space of the representations for the structure of the representations themselves are not explicit in the case of symplectic or orthogonal groups of order less than $Sp(4) \cong SO(5)$, since $Sp(2) \cong SO(3) \cong SU(2)$ and $SO(4) \cong SU(2) \otimes SU(2)$. The representation theory of the unitary groups has been extensively studied in terms of that of the symmetric groups. This method was initiated by Weyl[14] and extended by Schwinger,[16] Bargmann,[17] Friedrichs,[18] Moshinsky,[19,20] and Baird and Biedenharn,[21] who noted that the p vectors of the carrier space B may be mapped onto the boson creation operators $A_i^j \rightleftarrows a_i^j$, where the superscript j takes on values from 1 to p and the subscript i, from 1 to n. The boson operators obey the commutation rules $[\bar{a}_i^j, a_{i'}^{j'}] = \delta_{ii'}\delta_{jj'}$, with all other commutators equal to zero; here $\bar{a}$ denotes the destruction operator, the Hermitian conjugate of a. As usual $\langle 0|\, a_i = \bar{a}_i\, |0\rangle = 0$. When we apply the Young symmetrizer to B and project out a particular symmetry type, then symmetrization is not necessary because of the boson nature of the a_i^j. A particular state of an irreducible representation then becomes the product of boson operators a_i^1 and the antisymmetrized combinations

$$a_{i_1 i_2 \cdots i_k} = \sum_{\text{perm}} \epsilon(i_1 i_2 \cdots i_k) a_{i_1}^1 a_{i_2}^2 \cdots a_{i_k}^k. \quad (1.1)$$

A "state in the Weyl basis" is then given by such a product, in which each antisymmetrized product of the form (1.1), with $k \geq 2$, represents a column of the Young pattern with k nodes, and the bosons a_i^1 represent columns which consist of only a single node. These states of the Weyl basis are not mutually orthogonal. The mutually orthonormal states of the Gel'fand basis, however, can be expanded in terms of states of the Weyl basis, and these expansions have been studied extensively for the unitary groups by Baird and Biedenharn,[21] and by Ciftan.[22,23] For

[12] J. S. Lomont and H. E. Moses, J. Math. Phys. **5**, 294 (1964).
[13] J. S. Lomont and H. E. Moses, J. Math. Phys. **5**, 1438 (1964).
[14] H. Weyl, *Classical Groups* (Princeton University Press, Princeton, N.J., 1946).
[15] M. Hamermesh, *Group Theory* (Addison-Wesley Publ. Co., Inc., Reading, Mass., 1962).
[16] J. Schwinger, "On Angular Momentum," in *Quantum Theory of Angular Momentum*, L. C. Biedenharn and H. Van Dam, Eds. (Academic Press Inc., New York, 1965).
[17] V. Bargmann, Commun. Pure Appl. Math. **14**, 198 (1961).
[18] K. O. Friedrichs, *Mathematical Aspects of the Quantum Theory of Fields* (Interscience Publishers, Inc., New York, 1953).
[19] M. Moshinsky, Nucl. Phys. **31**, 384 (1962).
[20] M. Moshinsky, Rev. Mod. Phys. **34**, 813 (1962).
[21] G. Baird and L. C. Biedenharn, J. Math. Phys. **4**, 1449 (1963).
[22] M. Ciftan, thesis, Duke University, Durham, N.C., 1967 (unpublished).
[23] M. Ciftan, J. Math. Phys. **10**, 1639 (1969).

$U(2)$ the states of the Gel'fand basis are given by

$$\left|\begin{pmatrix} m_{12} & & m_{22} \\ & m_{11} & \end{pmatrix}\right\rangle = \mathcal{M}_2^{-\frac{1}{2}}(a_{12})^{m_{22}}(a_1^1)^{m_{11}-m_{22}}(a_2^1)^{m_{12}-m_{11}}|0\rangle, \tag{1.2}$$

while for $U(3)$ we have

$$\left|\begin{pmatrix} m_{13} & & m_{23} & & m_{33} \\ & m_{12} & & m_{22} & \\ & & m_{11} & & \end{pmatrix}\right\rangle = \mathcal{M}_3^{-\frac{1}{2}}(a_{123})^{m_{33}}(a_{12})^{m_{22}-m_{33}}(a_{13})^{m_{23}-m_{22}}(a_1^1)^{m_{11}-m_{23}}(a_2^1)^{m_{12}-m_{11}}(a_3^1)^{m_{13}-m_{12}}$$

$$\times {}_2F_1\left(m_{22}-m_{23}, m_{11}-m_{12}\,|m_{11}-m_{23}+1|\left(\frac{a_1^1 a_{23}}{a_2^1 a_{13}}\right)\right)|0\rangle, \tag{1.3}$$

and we shall henceforth abbreviate $a_i^1 = a_i$. The constants $\mathcal{M}^{-\frac{1}{2}}$ are constants of normalization which can be calculated by combinatorial methods. The expression of the expansion (1.3) in terms of a hypergeometric function is not just a convenient symbolism, as we frequently need the Kummer transformations and the contiguity relations of the ${}_2F_1$ functions, e.g., in the expressions for the matrix elements of the generators, etc. The corresponding expansions for higher unitary groups have been studied by Ciftan from the standpoint of combinatorial theory; he has discovered a general procedure for the derivation of the boson expansion for all of the $U(n)$ groups and has written it down explicitly for $U(4)$. The functions involved are generalizations of the hypergeometric series, but unfortunately they are neither Lauricella nor Appell series nor, in fact, any of the generalizations which have yet been studied. They are products of the constituents of hypergeometric functions on several variables, each such function being a Radon transform of linear forms. The totality of the expression of $U(4)$ states is then a "contracted" or "folded" form over the constituents of such transforms.

In the present work we shall study the extension of the method of the boson calculus to $Sp(4)$, which is the spinor covering group of $SO(5)$. This group has been studied by Hecht,[24] and more recently by Kemmer, Pursey, and Williams,[25,26] and by Sharp and Pieper[27]; it is the lowest of the symplectic or orthogonal groups which exhibits their algebraic peculiarities. It is hoped that the methods employed here may eventually be extended to all the symplectic and orthogonal groups. In Sec. 2 we study the restriction of the boson operators of $SU(4)$ to the representation space of $Sp(4)$, and we use the lowering operators of the group derived by Hecht in order to find the expression for a general state of an $Sp(4)$ representation in terms of the boson operators. Alternative forms of this expression are given. In Sec. 3 we use the basis states so constructed in order to derive the matrix elements of a finite rotation in five dimensions. It is found that these matrix elements can be expressed simply in terms of the representation functions and 9-j coefficients of $SU(2)$ by means of an interesting application of the Regge symmetries of the $SU(2)$ Wigner coefficients.[28] The second contribution of this paper, then, is this construction of all the irreducible unitary representation functions of $SO(5)$. The corresponding functions for $SO(4)$ have been studied by Dolginov[29] and by Biedenharn.[30] Those of $SO(3, 1)$ have been treated by a number of authors,[31–36] but for the compact and noncompact rotation groups in more than four dimensions only the functions of the most degenerate series have been obtained, at least to the best of the present author's knowledge.[37–40]

2. BASIS STATES FOR IRREDUCIBLE UNITARY REPRESENTATIONS OF $SP(4)$

The Lie algebra of $Sp(4)$ and $SO(5)$, and the states of their irreducible representations have been studied by Hecht,[24] who has also constructed the general

[24] K. T. Hecht, Nucl. Phys. **63**, 177 (1965).
[25] N. Kemmer, D. L. Pursey, and S. A. Williams, J. Math. Phys. **9**, 1224 (1968).
[26] S. A. Williams and D. L. Pursey, J. Math. Phys. **9**, 1230 (1968).
[27] R. T. Sharp and S. C. Pieper, J. Math. Phys. **9**, 663 (1968).
[28] T. Regge, Nuovo Cimento **10**, 544 (1958).
[29] A. Z. Dolginov, Soviet Phys.—JETP **3**, 589 (1956).
[30] L. C. Biedenharn, J. Math. Phys. **2**, 433 (1961).
[31] A. Z. Dolginov and I. N. Toptygin, Zh. Eksp. Teor. Fiz. **35**, 794 (1958) [Sov. Phys.—JETP **8**, 550 (1959)].
[32] A. Z. Dolginov and A. N. Moskalev, Sov. Phys.—JETP **10**, 1202 (1960).
[33] L. D. Eskin, Izv. Vysshikh Ucheb. Zavedeni Mat. **6**, (25), 179 (1961).
[34] S. Ström, Arkiv Fysik **29**, 467 (1965).
[35] Dao Wang Duc and Nguyen Van Hieu, Ann. Inst. Henri Poincaré **6**, 17 (1967).
[36] I. A. Verdiev and L. A. Dadashev, Institute of Theoretical and Experimental Physics, Preprint No. 476, 1966.
[37] J. Niederle and R. Rączka, ICTP Preprint IC/65/89, Trieste, 1965.
[38] R. Rączka, N. Limić, and J. Niederle, J. Math. Phys. **7**, 1861 (1966).
[39] N. Limić, J. Niederle, and R. Rączka, J. Math. Phys. **7**, 2026 (1966).
[40] N. Limić, J. Niederle, and R. Rączka, J. Math. Phys. **8**, 1079 (1967).

TABLE I. The 10 generators of the Lie algebra.

E_{ij}	L_{ij}
$\frac{1}{2}(E_{11}-E_{22})$	$\frac{1}{2}(L_{12}+L_{34})$
E_{12}	$\frac{1}{2}[(L_{23}+L_{14})+i(L_{31}+L_{24})]$
E_{21}	$\frac{1}{2}[(L_{23}+L_{14})-i(L_{31}+L_{24})]$
$\frac{1}{2}(E_{33}-E_{44})$	$\frac{1}{2}(L_{12}-L_{34})$
$-E_{34}$	$\frac{1}{2}[(L_{23}-L_{14})+i(L_{31}-L_{24})]$
$-E_{43}$	$\frac{1}{2}[(L_{23}-L_{14})-i(L_{31}-L_{24})]$
$\sqrt{\frac{1}{2}}(E_{14}+E_{32})$	$\sqrt{\frac{1}{2}}(L_{52}+iL_{15})$
$\sqrt{\frac{1}{2}}(E_{41}+E_{23})$	$\sqrt{\frac{1}{2}}(L_{52}-iL_{15})$
$\sqrt{\frac{1}{2}}(E_{13}-E_{42})$	$\sqrt{\frac{1}{2}}(L_{45}+iL_{53})$
$\sqrt{\frac{1}{2}}(E_{31}-E_{24})$	$\sqrt{\frac{1}{2}}(L_{45}-iL_{53})$

lowering operators for the group. The Lie algebra is spanned by 10 elements which are given in Table I [reproduced from Ref. 24], both in terms of the Weyl generators E_{ij} of the $SU(4)$ group, and in terms of the generators

$$L_{ij} = -i\left(x_i \frac{\partial}{\partial x_j} - x_j \frac{\partial}{\partial x_i}\right)$$

of rotations in the (ij) plane. The generators which are beside each other in the two columns are isomorphic. The Weyl generators have the commutation relations $[E_{ij}, E_{kl}] = E_{il}\delta_{jk} - E_{kj}\delta_{il}$ and are mapped onto the boson operators

$$E_{ij} \to \sum_p a_i^p \bar{a}_j^p. \tag{2.1}$$

The ten generators of $Sp(4)$, then, can be expressed as certain linear combinations of the sixteen generators of $SU(4)$. Since the irreducible representations of $Sp(4)$ correspond to Young diagrams of no more than two rows, we have it that we need use only the "single" boson operators a_i, $1 \leq i \leq 4$, and the "double" bosons a_{jk}, $1 \leq j, k \leq 4$, where

$$a_{jk} = a_j^1 a_k^2 - a_k^1 a_j^2. \tag{2.2}$$

In order to find which of these bosons actually occurs we must impose upon the carrier space B of the representation the condition that the symplectic trace vanish. A transformation of the group specified by the tensor product of two of the defining representations is given by

$$A_{j_1}^{(1)'} A_{j_2}^{(2)'} = S_{j_1}^{i_1} S_{j_2}^{i_2} A_{i_1}^{(1)} A_{i_2}^{(2)}, \tag{2.3}$$

and we must project out of the product $A_{i_1}^{(1)} A_{i_2}^{(2)}$ the subspace which has the symplectic trace equal to zero. Now the symplectic trace of $A_{i_1}^{(1)} A_{i_2}^{(2)}$ is given by $\epsilon_{i_1 i_2} A_{i_1}^{(1)} A_{i_2}^{(2)}$, where

$$\epsilon_{i_1 i_2} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{2.4}$$

Hence, the traceless part of $A_{i_1}^{(1)} A_{i_2}^{(2)}$ is given by

$$A_{i_1}^{(1)} A_{i_2}^{(2)} - \tfrac{1}{4}\epsilon_{i_1 i_2}[\epsilon_{j_1 j_2} A_{j_1}^{(1)} A_{j_2}^{(2)}] \equiv B_{i_1 i_2}^{(0)}. \tag{2.5}$$

We now apply the Young symmetrizer to $B_{i_1 i_2}^{(0)}$; taking the antisymmetric part of $B_{i_1 i_2}^{(0)}$ and mapping onto the boson operators, we find that the admissible "double" bosons in our calculus are

$$\begin{aligned} a_{12}^{(0)} &= a_1^1 a_2^2 - \tfrac{1}{4}\epsilon_{12}[\epsilon_{j_1 j_2} a_{j_1}^1 a_{j_2}^2] - a_2^1 a_1^2 + \tfrac{1}{4}\epsilon_{21}[\epsilon_{j_1 j_2} a_{j_1}^1 a_{j_2}^2] \\ &= \tfrac{1}{2}(a_1^1 a_2^2 - a_2^1 a_1^2 - a_3^1 a_4^2 + a_4^1 a_3^2) \\ &= \tfrac{1}{2}(a_{12} - a_{34}) \equiv \tfrac{1}{2}b, \\ a_{34}^{(0)} &= \tfrac{1}{2}(a_{34} - a_{12}) = -\tfrac{1}{2}b, \\ a_{13}^{(0)} &= a_{13}, \\ a_{14}^{(0)} &= a_{14}, \\ a_{23}^{(0)} &= a_{23}, \\ a_{24}^{(0)} &= a_{24}. \end{aligned} \tag{2.6}$$

Hence, our boson calculus for the representations of $Sp(4)$ consists only of the bosons and their linear combinations given in (2.6) as well as the "single" bosons a_1, a_2, a_3, a_4. It may easily be verified that the bosons (2.6) are closed under commutation with the generators given in Table I.

The irreducible unitary representations of $Sp(4)$ are uniquely labeled by the maximal weights, i.e., the eigenvalues of the two diagonal generators $\frac{1}{2}(E_{11} - E_{22})$ and $\frac{1}{2}(E_{33} - E_{44})$; we shall denote these two maximal weights as J_m and Λ_m, respectively, in accordance with Hecht's notation. We shall further suppose that the representation space of the irreducible unitary representation (J_m, Λ_m) is reduced by the representations of the subgroup $SU(2) \otimes SU(2)$, where the two $SU(2)$ subgroups have the generators $\frac{1}{2}(E_{11} - E_{22})$, E_{12}, E_{21}, and $\frac{1}{2}(E_{33} - E_{44})$, $-E_{34}, -E_{43}$, respectively, and their representations are labeled by the angular momentum states (J, M_J) and (Λ, M_Λ). The magnetic quantum numbers $M_J[M_\Lambda]$ are eigenvalues of $\frac{1}{2}(E_{11} - E_{22})[\frac{1}{2}(E_{33} - E_{44})]$, and their maximal values in the irreducible representation $M_J = J_m\,[M_\Lambda = \Lambda_m]$ occur with unit multiplicity. Hence a state of the irreducible representation (J_m, Λ_m) is given by $|J_m, \Lambda_m; J, \Lambda; M_J, M_\Lambda\rangle$.

The state $|J_m, \Lambda_m; J_m, \Lambda_m; J_m, \Lambda_m\rangle$ of maximal weight corresponds to the Weyl pattern in which the boxes of the Young frame are filled with ones in the top row and threes in the bottom row, as is evident from the diagonal generators. Hence in terms of our boson calculus the state of maximal weight is given by $(a_{13})^{2\Lambda_m} a_1^{2\Delta}\,|0\rangle$, where $2\Delta = 2J_m - 2\Lambda_m$. With the

normalizing factor we have it that

$$|\max\rangle = |J_m, \Lambda_m; J_m, \Lambda_m; J_m, \Lambda_m\rangle = \left[\frac{(2\Delta+1)}{(2J_m+1)!\,(2\Lambda_m)!}\right]^{\frac{1}{2}} a_{13}^{2\Lambda_m} a_1^{2\Delta}\,|0\rangle. \quad (2.7)$$

Hecht has found the operators which, when operating on a state maximal in the $SU(2) \otimes SU(2)$ subgroup, i.e., a state $|J_m, \Lambda_m; J, \Lambda; J, \Lambda\rangle$, change J and Λ by $\frac{1}{2}$. These operators are

$$O_{-+} = E_{21}(E_{14} + E_{32}) + (E_{31} - E_{24})(E_{11} - E_{22} + 1), \quad (2.8a)$$

$$O_{--} = E_{43}O_{-+} + [E_{21}(E_{13} - E_{42}) - (E_{41} + E_{23}) \times (E_{11} - E_{22} + 1)] \times (E_{33} - E_{44} + 1), \quad (2.8b)$$

and they have the properties

$$O_{-+}\,|J_m, \Lambda_m; J, \Lambda; J, \Lambda\rangle = c\,|J_m, \Lambda_m; J - \tfrac{1}{2}, \Lambda + \tfrac{1}{2}; J - \tfrac{1}{2}, \Lambda + \tfrac{1}{2}\rangle, \quad (2.9a)$$

$$O_{--}\,|J_m, \Lambda_m; J, \Lambda; J, \Lambda\rangle = c'\,|J_m, \Lambda_m; J - \tfrac{1}{2}, \Lambda - \tfrac{1}{2}; J - \tfrac{1}{2}, \Lambda - \tfrac{1}{2}\rangle, \quad (2.9b)$$

$$[O_{--}, O_{-+}] = 0. \quad (2.10)$$

We may then apply E_{21} and E_{43}, respectively, to lower M_J and M_Λ from their maximal to general values. A general state $|J_m, \Lambda_m; J, \Lambda; M_J, M_\Lambda\rangle$, then, is given by the expression

$$|J_m, \Lambda_m; J, \Lambda; M_J, M_\Lambda\rangle = \mathcal{N}^{-\frac{1}{2}} E_{21}^{x}(-E_{43})^{y} O_{--}^{m} O_{-+}^{n} a_{13}^{2\Lambda_m} a_1^{2\Delta}\,|0\rangle, \quad (2.11)$$

where

$$\begin{aligned} J &= J_m - \tfrac{1}{2}n - \tfrac{1}{2}m, & 0 \le n \le 2\Delta, \\ \Lambda &= \Lambda_m + \tfrac{1}{2}n - \tfrac{1}{2}m, & 0 \le m \le 2\Lambda_m, \\ M_J &= J - x, & 0 \le x \le 2J, \\ M_\Lambda &= \Lambda - y, & 0 \le y \le 2\Lambda. \end{aligned} \quad (2.12)$$

The normalization constant has also been found by Hecht to be

$$\mathcal{N}^{-\frac{1}{2}} = \left[\frac{(2\Delta+1)!\,(J_m + \Lambda_m + J - \Lambda + 1)!\,(J_m - \Lambda_m + J + \Lambda + 1)!\,(J_m - \Lambda_m + J - \Lambda)!}{[(2J_m+1)!]^4[(2\Lambda_m)!]^2[(2\Delta)!]^2(J_m - \Lambda_m - J + \Lambda)!\,(J_m + \Lambda_m - J - \Lambda)!} \times \frac{(\Lambda_m - J_m + J + \Lambda)!\,(J_m + \Lambda_m + J + \Lambda + 2)!\,(2J+1)!\,(2\Lambda+1)!\,(J+M_J)!\,(\Lambda+M_\Lambda)!}{(2J_m + 2\Lambda_m + 2)!\,(J_m + \Lambda_m - J + \Lambda + 1)!\,(2J)!\,(2\Lambda)!\,(J-M_J)!\,(\Lambda - M_\Lambda)!}\right]^{\frac{1}{2}}. \quad (2.13)$$

We shall denote the normalization constant for the semimaximal state $M_J = J$, $M_\Lambda = \Lambda$ by $\mathcal{N}_{\mathrm{sm}}^{-\frac{1}{2}}$. We may now project out a state of the subgroup of rotations in the three dimensions (123) by means of the coupling

$$|J_m, \Lambda_m; J, \Lambda; L, M\rangle = \sum_{M_J, M_\Lambda} C^{J}_{M_J}{}^{\Lambda}_{M_\Lambda}{}^{L}_{M}\,|J_m, \Lambda_m; J, \Lambda; M_J, M_\Lambda\rangle. \quad (2.14)$$

Since the operators O_{--} and O_{-+} commute with one another, the order in which they are applied to the maximal state is arbitrary. Tedious but straightforward inductions give us the following results:

$$O_{-+}^{n}(a_{13})^{2\Lambda_m} a_1^{2\Delta}\,|0\rangle = \frac{(2J_m+1)!}{(2J_m - n + 1)!}\,\frac{(2\Delta)!}{(2\Delta - n)!}\,(a_{13})^{2\Lambda_m} a_1^{2\Delta}\left(\frac{a_3}{a_1}\right)^{n}|0\rangle; \quad (2.15)$$

$$O_{--}^{m}(a_{13})^{2\Lambda_m} a_1^{2\Delta}\,|0\rangle = \sum_{\ell,d,h,k} (-1)^{m-\ell+h+k}\,\frac{(2\Lambda_m)!\,m!}{(2\Lambda_m - m)!}\,\frac{(2J_m+1)!}{(2J_m - m + 1)!}\,\frac{(2\Lambda_m + 1)!\,(2\Delta)!}{(2\Lambda_m - m + \ell + h + d + 1)!} \times \frac{1}{d!\,h!\,(2\Delta - h - k)!}\,\frac{1}{k!\,(\ell - k)!\,(m - 2\ell - 2d - h + k)!}\,(a_{13})^{2\Lambda_m} \times a_1^{2\Delta}\left(\frac{b}{a_{13}}\right)^{m}\left(\frac{a_{13}a_{24}}{b^2}\right)^{\ell}\left(\frac{a_{14}a_{23}}{b^2}\right)^{d}\left(\frac{a_{14}a_3}{ba_1}\right)^{h}\left(\frac{ba_4}{a_{24}a_1}\right)^{k}|0\rangle; \quad (2.16)$$

where the boundaries of the summations in the four-dimensional lattice of the indices ℓ, d, h, and k are given by the zeros of the factorials in the denominator. This expression may be simplified if we write it in terms of a_{12} and a_{34} rather than b:

$$\frac{(2\Lambda_m)!\,[(2J_m+1)!]^2}{(2\Lambda_m - m)!\,[(2J_m - m + 1)!]^2}\,{}_2F_1\left(-m, -2\Lambda_m - 1\,|2J_m - m + 2|\,-\frac{a_{12}}{a_{34}}\right)\left(\frac{a_{34}}{a_{13}}\right)^{m} a_{13}^{2\Lambda_m} a_1^{2\Delta}\,|0\rangle. \quad (2.16')$$

Applying both O_{--}^{m} and O_{-+}^{n} to the maximal state we find

$$O_{--}^{m}O_{-+}^{n}(a_{13})^{2\Lambda_m} a_1^{2\Delta}\,|0\rangle = \sum_{\ell,d,g,h,k} (-1)^{m+n-\ell+h+k}\,\frac{(2\Lambda_m)!\,m!}{(2\Lambda_m - m)!}\,\frac{(2J_m+1)!}{(2J_m - m + 1)!}\,\frac{(2\Lambda_m + n + 1)!\,(2\Delta)!\,n!}{(2\Lambda_m - m + \ell + h + d + 1)!}$$

$$\times \frac{1}{h!\,g!\,k!\,(\ell-k-g)!\,(m+n-2\ell-2d-h+k)!\,(n-g)!}\,\frac{1}{(d-n+g)!\,(2\Delta-h-k-n)!}$$
$$\times {}_3F_2(-n+g,\,2J_m-m-n+\ell+d-k+2,\,-h\,|d-n+g+1,\,2\Delta-h-k-n+1|\,1)$$
$$\times (a_{13})^{2\Lambda_m}a_1^{2\Delta}\left(\frac{b}{a_{13}}\right)^m\left(\frac{b}{a_{14}}\right)^n\left(\frac{a_{13}a_{24}}{b^2}\right)^\ell\left(\frac{a_{14}a_{23}}{b^2}\right)^d\left(\frac{a_{14}a_3}{ba_1}\right)^h\left(\frac{ba_4}{a_{24}a_1}\right)^k\left(\frac{a_{14}a_2}{a_{24}a_1}\right)^g|0\rangle$$
$$=\frac{(2\Lambda_m)!\,[(2J_m+1)!]^2(2\Delta)!}{(2\Lambda_m-m)!\,(2J_m-m+1)!\,(2\Delta-n)!\,(2J_m-m-n+1)!}$$
$$\times {}_2F_1\left(-m,\,-2\Lambda_m-n-1\,|2J_m-m-n+2|\,-\frac{a_{12}}{a_{34}}\right)\left(\frac{a_{34}}{a_{13}}\right)^m\left(\frac{a_3}{a_1}\right)^n a_{13}^{2\Lambda_m}a_1^{2\Delta}|0\rangle. \tag{2.17}$$

Multiplying (2.17) by $\mathcal{M}_{\rm sm}^{-\frac{1}{2}}$, we find that the normalized semimaximal state can be written as

$$\mathcal{M}_{\rm sm}^{-\frac{1}{2}}\frac{(J_m+\Lambda_m-J-\Lambda)!\,(J_m+\Lambda_m-J+\Lambda+1)!\,[(2J_m+1)!]^2(2\Lambda_m)!\,(2\Delta)!}{(J_m-\Lambda_m+J-\Lambda)!\,(2J+1)!\,(2\Lambda+1)!}$$
$$\times\sum_{\substack{j_1j_2\\ m_1m_2\\ \mu_1\mu_2}}(-1)^{2j_2}\Bigg[\frac{(J+j_1-j_2)!\,(\Lambda+\lambda_1-\lambda_2)!}{(J+j_2-j_1)!\,(j_1+j_2-J)!\,(J+j_1+j_2+1)!\,(\Lambda+\lambda_2-\lambda_1)!\,(\lambda_1+\lambda_2-\Lambda)!}$$
$$\times\frac{1}{(\Lambda+\lambda_1+\lambda_2+1)!}\Bigg]^{\frac{1}{2}}C^{j_1\ j_2\ J}_{m_1\ m_2\ J}C^{\lambda_1\ \lambda_2\ \Lambda}_{\mu_1\ \mu_2\ \Lambda}\left(\frac{(a_1^1)^{j_1+m_1}(a_2^1)^{j_1-m_1}}{[(j_1+m_1)!\,(j_1-m_1)!]^{\frac{1}{2}}}\right)$$
$$\times\left(\frac{(a_1^2)^{j_2+m_2}(a_2^2)^{j_2-m_2}}{[(j_2+m_2)!\,(j_2-m_2)!]^{\frac{1}{2}}}\right)\left(\frac{(a_3^1)^{\lambda_1+\mu_1}(a_4^1)^{\lambda_1-\mu_1}}{[(\lambda_1+\mu_1)!\,(\lambda_1-\mu_1)!]^{\frac{1}{2}}}\right)\left(\frac{(a_3^2)^{\lambda_2+\mu_2}(a_4^2)^{\lambda_2-\mu_2}}{[(\lambda_2+\mu_2)!\,(\lambda_2-\mu_2)!]^{\frac{1}{2}}}\right)|0\rangle$$
$$\equiv\sum_{\substack{j_1j_2\\ m_1m_2\\ \mu_1\mu_2}}\mathcal{F}(J_m\Lambda_m;\,J\Lambda;\,j_1j_2)C^{j_1\ j_2\ J}_{m_1\ m_2\ J}C^{\lambda_1\ \lambda_2\ \Lambda}_{\mu_1\ \mu_2\ \Lambda}\left(\frac{(a_1^1)^{j_1+m_1}(a_2^1)^{j_1-m_1}}{[(j_1+m_1)!\,(j_1-m_1)!]^{\frac{1}{2}}}\right)$$
$$\times\left(\frac{(a_1^2)^{j_2+m_2}(a_2^2)^{j_2-m_2}}{[(j_2+m_2)!\,(j_2-m_2)!]^{\frac{1}{2}}}\right)\left(\frac{(a_3^1)^{\lambda_1+\mu_1}(a_4^1)^{\lambda_1-\mu_1}}{[(\lambda_1+\mu_1)!\,(\lambda_1-\mu_1)!]^{\frac{1}{2}}}\right)\left(\frac{(a_3^2)^{\lambda_2+\mu_2}(a_4^2)^{\lambda_2-\mu_2}}{[(\lambda_2+\mu_2)!\,(\lambda_2-\mu_2)!]^{\frac{1}{2}}}\right)|0\rangle, \tag{2.18}$$

where the j_i and the λ_i are not independent but are related by

$$j_1+\lambda_1=J_m,$$
$$j_2+\lambda_2=\Lambda_m. \tag{2.19}$$

In (2.18) the summations are carried out over all integral and half-integral values of j_1 and j_2 which are compatible with the couplings indicated by the $SU(2)$ Wigner coefficients. Henceforth we shall work exclusively with the simpler forms of these basis states which we obtain by decomposing the boson combination $b=a_{12}-a_{34}$; we give the more complicated expression for whatever interest it may have from the standpoint of combinatorial theory.

We now apply $E_{21}^x(-E_{43})^y$ to lower the magnetic quantum numbers from maximal to general values. We note that all the generators of the $Sp(2)\otimes Sp(2)\simeq SO(4)$ subgroup commute with a_{12} and a_{34}. Hence we obtain

$$E_{21}^x(-E_{43})^yO_{--}^mO_{-+}^na_{13}^{2\Lambda_m}a_1^{2\Delta}|0\rangle$$
$$=(-1)^y\frac{(2\Lambda_m)!\,[(2J_m+1)!]^2n!}{(2J_m-m+1)!\,(2J_m-m-n+1)!}(2\Delta)!\,x!\,y!$$
$$\times\sum_{k_1z_1z_2}\frac{1}{k_1!\,(2\Delta-n-k_1)!\,z_1!\,(n-z_1)!\,z_2!\,(2\Lambda_m-m-x+k_1-z_2)!}$$
$$\times\frac{1}{(y-z_1-z_2)!\,(x-k_1-y+z_1+z_2)!}\,{}_2F_1\left(-m,\,-2\Lambda_m-n-1\,|2J_m-m-n+2|\,-\frac{a_{12}}{a_{34}}\right)$$
$$\times\left(\frac{a_{34}}{a_{13}}\right)^m\left(\frac{a_3}{a_1}\right)^n\left(\frac{a_{23}}{a_{13}}\right)^x\left(\frac{a_{24}}{a_{23}}\right)^y\left(\frac{a_{13}a_2}{a_{23}a_1}\right)^{k_1}\left(\frac{a_{23}a_4}{a_{24}a_3}\right)^{z_1}\left(\frac{a_{14}a_{23}}{a_{13}a_{24}}\right)^{z_2}a_{13}^{2\Lambda_m}a_1^{2\Delta}|0\rangle, \tag{2.20}$$

which is normalized by the factor (2.13). Applying the normalized lowering operators to the expression (2.18),

we may write the normalized general state immediately as

$$|J_m\Lambda_m; J, \Lambda; M_J, M_\Lambda\rangle = (-1)^{\Lambda-M_\Lambda} \sum_{\substack{j_1 j_2 m_1 m_2 \\ \mu_1 \mu_2}} \mathcal{F}(J_m\Lambda_m; J\Lambda; j_1 j_2) \times C^{j_1\ j_2\ J}_{m_1\ m_2\ M_J} C^{\lambda_1\ \lambda_2\ \Lambda}_{\mu_1\ \mu_2\ M_\Lambda} \left(\frac{(a_1^1)^{j_1+m_1}(a_2^1)^{j_1-m_1}}{[(j_1+m_1)!\,(j_1-m_1)!]^{\frac{1}{2}}}\right)\left(\frac{(a_1^2)^{j_2+m_2}(a_2^2)^{j_2-m_2}}{[(j_2+m_2)!\,(j_2-m_2)!]^{\frac{1}{2}}}\right) \times \left(\frac{(a_3^1)^{\lambda_1+\mu_1}(a_4^1)^{\lambda_1-\mu_1}}{[(\lambda_1+\mu_1)!\,(\lambda_1-\mu_1)!]^{\frac{1}{2}}}\right)\left(\frac{(a_3^2)^{\lambda_2+\mu_2}(a_4^2)^{\lambda_2-\mu_2}}{[(\lambda_2+\mu_2)!\,(\lambda_2-\mu_2)!]^{\frac{1}{2}}}\right)|0\rangle, \tag{2.21}$$

from which we may project the angular momentum state of the $SO(3)$ subgroup by means of the coupling (2.14). We shall henceforth deal with this latter basis exclusively.

III. MATRIX ELEMENTS OF FINITE ROTATIONS IN FIVE DIMENSIONS

We may parametrize the group of rotations in five dimensions in the following manner:

$$(R_5) = (R_4)e^{iL_{45}\theta}(R_4), \tag{3.1}$$

where (R_4) denotes a transformation of the subgroup of rotations in four dimensions [the dimensions labeled in the Table above by the indices (1234)], and L_{45} is the generator of rotations in the (45) plane. The representation functions of $SO(4)$ are well known due to the work of Dolginov[29] and of Biedenharn,[30] so we need find only the matrix elements

$$\langle J_m\Lambda_m; J', \Lambda'; L', M'|\, e^{iL_{45}\theta}\,|J_m\Lambda_m; J, \Lambda; L, M\rangle. \tag{3.2}$$

Obviously both L_{45} and the matrix elements of finite rotations in the (45) plane are diagonal in L and M. This property will become explicit in the structure of the matrix elements (3.2).

In terms of our boson operators,

$$\begin{aligned} L_{45} &= \tfrac{1}{2}(E_{13} + E_{31} - E_{24} - E_{42}) \\ &= \tfrac{1}{2}\sum_{p=1}^{2}(a_1^p\bar{a}_3^p + a_3^p\bar{a}_1^p - a_2^p\bar{a}_4^p - a_4^p\bar{a}_2^p) \\ &= \sum_{p=1}^{2} L_{45}^{(p)}. \end{aligned} \tag{3.3}$$

Expanding

$$e^{iL_{45}\theta} = \sum_{n=0}^{\infty}\frac{(iL_{45}\theta)^n}{n!} \tag{3.4}$$

and operating on the state $B = A_{i_1}^{(1)}A_{i_2}^{(2)}$, we have

$$e^{iL_{45}\theta} = e^{iL_{45}^{(1)}\theta}A^{(1)}e^{iL_{45}^{(2)}\theta}A^{(2)} = \prod_{p=1}^{2}\left[\begin{pmatrix} \cos\frac{1}{2}\theta & 0 & i\sin\frac{1}{2}\theta & 0 \\ 0 & \cos\frac{1}{2}\theta & 0 & -i\sin\frac{1}{2}\theta \\ i\sin\frac{1}{2}\theta & 0 & \cos\frac{1}{2}\theta & 0 \\ 0 & -i\sin\frac{1}{2}\theta & 0 & \cos\frac{1}{2}\theta \end{pmatrix}\begin{pmatrix} A_1^{(p)} \\ A_2^{(p)} \\ A_3^{(p)} \\ A_4^{(p)} \end{pmatrix}\right]. \tag{3.5}$$

This relation prescribes that the expression

$$e^{iL_{45}\theta}\,|J_m\Lambda_m; J, \Lambda; L, M\rangle \tag{3.6}$$

is given by the normalized basis state with the replacements

$$\begin{pmatrix} a_1^p \\ a_2^p \\ a_3^p \\ a_4^p \end{pmatrix} \to \begin{pmatrix} \cos\frac{1}{2}\theta a_1^p + i\sin\frac{1}{2}\theta a_3^p \\ \cos\frac{1}{2}\theta a_2^p - i\sin\frac{1}{2}\theta a_4^p \\ i\sin\frac{1}{2}\theta a_1^p + \cos\frac{1}{2}\theta a_3^p \\ -i\sin\frac{1}{2}\theta a_2^p + \cos\frac{1}{2}\theta a_4^p \end{pmatrix}. \tag{3.7}$$

This suggests that we may write down the matrix elements (3.2) in terms of $SU(2)$ representation functions $\mathcal{d}^j_{m'm}(\theta)$ corresponding to rotations about the x axis in the isomorphic $SO(3)$ case if we regroup the bosons in (2.21) into a different set of four angular momenta. That is, we wish to form angular momentum states with the boson groupings $(a_1^p a_3^p)$ and $(a_2^p a_4^p)$ rather than the groupings $(a_1^p a_2^p)$ and $(a_3^p a_4^p)$ indicated in (2.21), which were chosen because of their invariance under the generators of the $Sp(2) \otimes Sp(2)$ subgroup. We shall find that this "restitching" of the constituent angular momentum states can easily be expressed when we invoke the Regge symmetries of the $SU(2)$ Wigner coefficients.[28]

Let us consider initial and final states of the form (2.21) with the coupling (2.14). For the final state all quantum numbers and summation indices will be denoted by the corresponding primed quantities. Let us also momentarily suppress the coefficients of the four normalized $Sp(2)$ angular momentum states on the right of (2.21). It immediately follows that we may write the function (3.2) as an expansion in terms of the form

$$\prod_{i=1}^{2} \mathcal{d}^{\frac{1}{2}(j_i+\lambda_i+m_i+\mu_i)}_{\frac{1}{2}(j_i'-\lambda_i'+m_i'-\mu_i')\,\frac{1}{2}(j_i-\lambda_i+m_i-\mu_i)}(\theta) \times \mathcal{d}^{\frac{1}{2}(j_i+\lambda_i-m_i-\mu_i)}_{\frac{1}{2}(j_i'-\lambda_i'-m_i'+\mu_i')\,\frac{1}{2}(j_i-\lambda_i-m_i+\mu_i)}(-\theta)\delta_{m_i'+\mu_i',\,m_i+\mu_i}, \tag{3.8}$$

where the rotation functions $\mathcal{d}^j_{m'm}(\theta)$ are given in terms of the real $d^j_{m'm}(\theta)$ functions [for rotations about the y axis in $SO(3)$] by the relation

$$\mathcal{d}^j_{m'm}(\theta) = (i)^{m'-m}\, d^j_{m'm}(\theta), \tag{3.9}$$

and we follow the conventions of Edmonds for the $d^j_{m'm}(\theta)$ functions.[41] We now apply the symmetry

$$d^j_{m'm}(-\theta) = (-1)^{m'-m} d^j_{m'm}(\theta) \tag{3.10}$$

to the expression (3.8) and couple the two rotation functions in the standard way by means of $SU(2)$ Wigner coefficients. It is at this point that we invoke the Regge symmetries of these coefficients. We note that by Regge symmetry

$$C^{\frac{1}{2}(j_i+\lambda_i+m_i+\mu_i)\ \frac{1}{2}(j_i+\lambda_i-m_i-\mu_i)\ K_i}_{\frac{1}{2}(j_i-\lambda_i+m_i-\mu_i)\ \frac{1}{2}(j_i-\lambda_i-m_i+\mu_i)\ j_i-\lambda_i} = C^{j_i\ \lambda_i\ K_i}_{m_i\ \mu_i\ M_i}, \tag{3.11}$$

hence (3.8) becomes

$$(-1)^{\frac{1}{2}(M_J-M_\Lambda-M_{J'}+M_{\Lambda'})} \prod_{i=1}^{2} \sum_{K_i} (-1)^{\frac{1}{2}(j_{i'}-j_i+\lambda_i-\lambda_{i'})} \times C^{j_{i'}\ \lambda_{i'}\ K_i}_{m_{i'}\ \mu_{i'}\ M_i} d^{K_i}_{j_{i'}-\lambda_{i'}\,j_i-\lambda_i}(\theta) C^{j_i\ \lambda_i\ K_i}_{m_i\ \mu_i\ M_i}. \tag{3.12}$$

From (2.14), (2.21), and (3.12), we find that the "initial" and "final" sides of the matrix element (3.2) each contain five $SU(2)$ Wigner coefficients. We may perform the summations over the magnetic quantum numbers m_1, m_2, μ_1, μ_2, M_J, M_Λ by means of the identity

$$\sum_{\substack{m_i\mu_i \\ M_J M_\Lambda}} C^{J\ \Lambda\ L}_{M_J\ M_\Lambda\ M} C^{j_1\ j_2\ J}_{m_1\ m_2\ M_J} C^{\lambda_1\ \lambda_2\ \Lambda}_{\mu_1\ \mu_2\ M_\Lambda} C^{j_1\ \lambda_1\ K_1}_{m_1\ \mu_1\ M_1} C^{j_2\ \lambda_2\ K_2}_{m_2\ \mu_2\ M_2} = [(2K_1+1)(2K_2+1)(2J+1)(2\Lambda+1)]^{\frac{1}{2}} C^{K_1\ K_2\ L}_{M_1\ M_2\ M} \begin{Bmatrix} j_1 & \lambda_1 & K_1 \\ j_2 & \lambda_2 & K_2 \\ J & \Lambda & L \end{Bmatrix}, \tag{3.13}$$

where we recall that the magnetic quantum numbers in the exponent of (-1) in (3.12) are canceled by phases of the form $(-1)^{\Lambda-M_\Lambda}$ and $(-1)^{\Lambda'-M_{\Lambda'}}$ as indicated in (2.21). We must include this phase factor in (2.21) when we perform the coupling (2.14), because (JM_J) and (ΛM_Λ) are states of the $Sp(2)$ subgroups generated, respectively, by the operators $[\frac{1}{2}(E_{11}-E_{22}), E_{12}, E_{21}]$ and $[\frac{1}{2}(E_{33}-E_{44}), -E_{34}, -E_{43}]$.

Using the identity (3.13) to perform summations over magnetic quantum numbers in the final state, we find that we are left with summations over M_1 and M_2 which may be performed easily:

$$\sum_{M_1 M_2} C^{K_1\ K_2\ L}_{M_1\ M_2\ M} C^{K_1\ K_2\ L'}_{M_1\ M_2\ M'} = \delta_{L,L'}\delta_{M,M'}; \tag{3.14}$$

hence, as expected, the matrix element (3.2) is diagonal in the angular momentum state (LM). We may now write down our final result. The matrix element (3.2) is equal to

$$(-1)^{\Lambda-\Lambda'} \sum_{\substack{j_1 j_2 j_1' j_2' \\ K_1 K_2}} (2K_1+1)(2K_2+1)\mathcal{F}(J_m\Lambda_m; J'\Lambda'; j_1' j_2') \times [(2J'+1)(2\Lambda'+1)]^{\frac{1}{2}} \begin{Bmatrix} j_1' & \lambda_1' & K_1 \\ j_2' & \lambda_2' & K_2 \\ J' & \Lambda' & L \end{Bmatrix} d^{K_1}_{j_1'-\lambda_1'\ j_1-\lambda_1}(\theta)\, d^{K_2}_{j_2'-\lambda_2'\ j_2-\lambda_2}(\theta) \times \mathcal{F}(J_m\Lambda_m; J\Lambda; j_1 j_2)[(2J+1)(2\Lambda+1)]^{\frac{1}{2}} \begin{Bmatrix} j_1 & \lambda_1 & K_1 \\ j_2 & \lambda_2 & K_2 \\ J & \Lambda & L \end{Bmatrix}, \tag{3.15}$$

where we have applied (3.9).

It is worthwhile to consider also the matrix elements of $\exp(iL_{35}\theta)$ for the following reason. The representation functions of the de Sitter group $Sp(2,2) \cong SO(4,1)$ may be reached from those of $Sp(4) \cong SO(5)$ by a process of analytic continuation in θ and in $(J_m + \Lambda_m + 1)$. Let us consider the $SO(4,1)$ group in which the time dimension is the dimension here labeled by the index 5. In this process the matrix elements of $\exp(iL_{45}\theta)$ and of $\exp(iL_{35}\theta)$ both become those of "Lorentz transformations" in de Sitter space. We may now take suitable asymptotic limits of these functions and contract them in the sense of Wigner and Inönü to representations of the Poincaré group in the $E(3)$ (helicity angular-momentum) basis. We contract the dimension 4 and leave the time dimension 5 and the three space dimensions (123). The matrix elements of $\exp(iL_{35}\theta)$ now become those of a Lorentz transformation along the 3 axis, whereas those of $\exp(iL_{45}\theta)$ become time translations. Hence we should consider both types of function. To take matrix elements of $\exp(iL_{35}\theta)$ we follow similar procedures, but in (3.8) we must replace the $d^j_{m'm}(\theta)$ with $d^j_{m'm}(\theta)$, and both functions have argument $+\theta$. Hence in (3.12) we again replace d^{K_i} with d^{K_i}, but we must omit the complicated phase factor. Hence, because of the phases $(-1)^{\Lambda-M_\Lambda}(-1)^{\Lambda'-M_{\Lambda'}}$ indicated in (2.21), we cannot perform the summations on the left of (3.13), and (3.14) is inapplicable. Thus, although $\exp(iL_{35}\theta)$ is diagonal in M, it is not diagonal in L, as is to be expected.

ACKNOWLEDGMENTS

The author would like to thank Dr. Behram Kurşunoğlu for his gracious hospitality at the Center for Theoretical Studies and Dr. C. A. Hurst for helpful discussions.

[41] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, N.J., 1957), p. 57.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Nonlinear Electrodynamics and General Relativity

R. PELLICER AND R. J. TORRENCE*
Department of Physics
Centro de Investigacion y de Estudios Avanzados del Instituto Politecnico Nacional
Apdo. Postal 14-740, *Mexico* 14, *D.F.*

(Received 17 January 1969)

A generalization of Born–Infeld nonlinear electrodynamics, due to Plebanski, is reformulated in the context of general relativity theory. A class of nonsingular, static, spherically symmetric solutions of the modified Einstein–Maxwell equations are given, corresponding to a point-charge source. The metric tensors of these solutions are shown to approach the Riesner–Nordstrom metric tensor at large distances from the source, if one makes the proper identification of mass.

1. INTRODUCTION

Experiment compels us to seek field equations for the vacuum electromagnetic field which are approximately linear. For simplicity it is generally assumed that they are exactly linear, and this assumption, combined with the desire for Lorentz invariance, leads to a unique action and unique field equations for the vacuum electromagnetic field.[1] These equations, Maxwell's equations, have proven adequate, to say the least, in describing experimental results at the classical level; however, from the theoretician's point of view the situation is not entirely satisfactory. Solving Maxwell's equations for a distribution of point charges results in a field which is divergent at the locations of the point charges. This is unattractive in its own right, and in addition results in an infinite total energy for the field.

Various attempts have been made to eliminate the above difficulty from the theory. Of particular interest to us is the attempt, by Born and Infeld,[2] based upon a new choice of vacuum field action which leads to nonlinear field equations (such an action is referred to in this paper as a "nonlinear" action). Having chosen a particular "nonlinear" action, Born and Infeld solved the resulting field equations for the static, spherically symmetric solution (SSS solution) corresponding to a point charge. As might be expected, the resulting field was significantly different from a coulomb field in the neighborhood of the point charge where the fields are most intense, and they found, in fact, that their field was finite everywhere, including the location of the point charge.

The SSS solution of the Born–Infeld theory, although finite everywhere, is, however, discontinuous at the center of symmetry. In addition, their choice of a "nonlinear" action, although different from the usual one, did not exhaust the possible choices consistent with Lorentz invariance. The possibility existed, therefore, that some different "nonlinear" action might be found which would make the SSS solution not only finite everywhere, but continuous everywhere. The generalization of the Born–Infeld electromagnetic field action to include all "reasonable" actions was considered by Plebanski,[3] who investigated the resulting theories in some detail. Among other things, Plebanski showed that there exists a wide class of "nonlinear" actions which lead to field equations possessing SSS solutions which were nonsingular and, in fact, continuous everywhere.

The purpose of this paper is to extend Plebanski's work to the general relativistic case. That is to say, we consider Einstein–Maxwell theory with, however, the Maxwell theory replaced by Plebanski's nonlinear generalization of Maxwell theory. We present an SSS solution of the Einstein–(nonlinear) Maxwell equations, including both a metric tensor and an electromagnetic field tensor, and we investigate some of its properties. In particular, we show that there exists a class of nonlinear, electromagnetic field theories for which the SSS solutions, including both the metric and the electromagnetic field tensors, are everywhere continuous. In order to achieve this, it is assumed that the parameter which measures the mass of the point sources of the electromagnetic field is equal to zero, which is consistent with the interpretation of the mass of a charged particle as a property of its field, rather than as a property of the point source. Also in accord with the above point of view is the introduction of an effective electromagnetic mass defined in terms of the asymptotic behavior of the related gravitation field. This effective electromagnetic mass can be identified in such a way that our SSS solutions approach, asymptotically, the well-known

* Present address: The University of Calgary, Department of Mathematics, Calgary, Alberta, Canada.

[1] L. Landau and E. Lifshitz, *The Classical Theory of Fields* (Addison-Wesley Publ. Co., Inc., Reading, Mass., 1951), 2nd ed.

[2] M. Born and L. Infeld, Proc. Roy. Soc. (London) **144**, 425 (1934).

[3] J. Plebanski, *Non-Linear Electrodynamics—A Study* (C.I.E.A. del I.P.N., Mexico City, 1966).

Riesner–Nordstrom solution of the Einstein–Maxwell equations.

In the following section, we briefly review the Born–Infeld and the Plebanski nonlinear electromagnetic field theories and introduce the basic equations of Einstein–(nonlinear) Maxwell theory. In Sec. 3, we solve our equations for an SSS solution and investigate the behavior of this solution for both large and small distances from the location of the point charge, in order to show that it is free from singularities, discontinuous, and asymptotically Riesner–Nordstrom. We summarize our results in a short concluding section.

2. EINSTEIN-ELECTROMAGNETIC THEORY

A. Nonlinear Electrodynamics in Minkowski Space

If we assume that the nonlinear electromagnetic field can be described[4] by a vector potential A_μ through

$$f_{\mu\nu} = 2A_{[\mu,\nu]}, \tag{2.1}$$

then it is well known[1] that $f_{\mu\nu}$ possesses just one independent invariant and one independent pseudo-invariant, which can be defined as

$$F \equiv \tfrac{1}{4} f_{\alpha\beta} f^{\alpha\beta}, \quad G \equiv \tfrac{1}{4} f_{\alpha\beta} {}^*f^{\alpha\beta}, \tag{2.2}$$

where

$${}^*f^{\alpha\beta} \equiv \tfrac{1}{2} i \epsilon^{\alpha\beta\gamma\delta} f_{\gamma\delta} \tag{2.3}$$

with $i = \sqrt{-1}$. If we wish our theory to be invariant under the Lorentz group, including reflections, we must choose a Lagrangian depending only on F and G^2. In order to obtain the Maxwell theory, one chooses

$$L = F, \tag{2.4}$$

while

$$L = 2[(1 + F - G^2)^{\frac{1}{2}} - 1] \tag{2.5}$$

is the Lagrangian considered by Born and Infeld. To start with, we assume only that

$$L = L(F, G^2). \tag{2.6}$$

In addition we impose the condition that for weak fields the nonlinear theory should approximate the linear theory. [This is true, for example, with the Lagrangian given by Eq. (2.5).]

Using this generalized Lagrangian, we now give the action for a system of point charges interacting with an electromagnetic field[1]:

$$W = -\sum_{a=1}^{N} m_a c \int_{\sigma_1}^{\sigma_2} dS_a + \sum_{a=1}^{N} \frac{e_a}{c} \int_{\sigma_1}^{\sigma_2} A_\alpha(a^\beta)\, da^\alpha - \frac{1}{4\pi c} \int_{\sigma_1}^{\sigma_2} L(F, G^2)\, d^4x. \tag{2.7}$$

In this expression the index a labels the N particles, a^α represents the world line of the ath particle, with m_a and e_a as its mass and charge, respectively, and S_a as the proper time of the ath particle. The last integral is over a world tube enclosing the particle world lines, and bounded at the ends by spacelike hypersurfaces σ^1 and σ^2, while the first two integrals are line integrals between the points of intersection of the particle world lines and the spacelike hypersurfaces.

The integrability conditions of Eq. (2.1) are known to be

$$({}^*f^{\alpha\beta})_{,\beta} = 0, \tag{2.8a}$$

which is our first set of field equations; setting $\delta W/\delta W_\alpha = 0$ yields

$$2\left(\frac{\partial L(F, G^2)}{\partial f_{\alpha\beta}}\right)_{,\beta} = 4\pi \sum_{a=1}^{N} e_a \int_{-\infty}^{+\infty} \delta_4(x^\alpha - a^\alpha)\, da^\alpha, \tag{2.8b}$$

which is our second set of field equations. Thus, Eqs. (2.8a) and (2.8b) are the generalization of Maxwell's equations, with Eqs. (2.8a) unchanged in form. If we set $\delta W/\delta a^\alpha = 0$, we get

$$m_a c \frac{d^2 a^\alpha}{dS_a^2} + \frac{e_a}{c} f^\alpha_\beta \frac{da^\beta}{dS_a} = 0, \tag{2.9}$$

which is the usual equation for the Lorentz force.

It is convenient to introduce the canonical formalism for the system as well. We define

$$p^{\alpha\beta} \equiv 2\frac{\partial L}{\partial f_{\alpha\beta}} = \frac{\partial L}{\partial F} f^{\alpha\beta} + \frac{\partial L}{\partial G} {}^*f^{\alpha\beta} \tag{2.10}$$

and

$$H \equiv \tfrac{1}{2} p^{\alpha\beta} f_{\alpha\beta} - L(F, G^2). \tag{2.11}$$

Substituting Eq. (2.10) into Eq. (2.11) gives

$$H = 2\left(\frac{\partial L}{\partial F} F + \frac{\partial L}{\partial G} G\right) - L(F, G^2) = H(F, G^2). \tag{2.12}$$

However, using Eq. (2.10), we can derive

$$P + Q = \left(\frac{\partial L}{\partial F} + \frac{\partial L}{\partial G}\right)^2 (F + G), \tag{2.13}$$

where

$$P \equiv \tfrac{1}{4} p_{\alpha\beta} p^{\alpha\beta}, \quad Q \equiv \tfrac{1}{4} p_{\alpha\beta} {}^*p^{\alpha\beta}, \tag{2.14}$$

and if Eq. (2.13) can be inverted to obtain $F(P, Q)$, $G(P, Q)$, then Eq. (2.12) yields

$$H = H(P, Q^2). \tag{2.15}$$

[4] Greek and Latin indices range from 0 to 3 and 1 to 3, respectively, while the metric has signature (+, −, −, −) (and in Sec. 2A only, is the Minkowski metric). Partial and covariant differentiation may be denoted by a comma and a semicolon, respectively. Finally, $\epsilon^{\alpha\beta\gamma\delta}$ is the alternating tensor density, and $|g_{\mu\nu}| \equiv g$.

Hamilton's equations are then

$$f^{\alpha\beta} = 2\frac{\partial H}{\partial p_{\alpha\beta}} = \frac{\partial H}{\partial P}p^{\alpha\beta} + \frac{\partial H}{\partial Q}{}^*p^{\alpha\beta} \quad (2.16)$$

and

$$(p^{\alpha\beta})_{,\beta} = 4\pi\sum_{a=1}^{N} e_a \int_{-\infty}^{+\infty} \delta_4(x^\alpha - a^\alpha)\, da^\alpha, \quad (2.17a)$$

and if we substitute Eq. (2.16) into Eq. (2.8a) to obtain

$$\left(\frac{\partial H}{\partial P}{}^*p^{\alpha\beta} + \frac{\partial H}{\partial Q}p^{\alpha\beta}\right)_{,\beta} = 0, \quad (2.17b)$$

we have the choice of working with either Eqs. (2.8) or Eqs. (2.17). Note that in both the Maxwell theory and the Born–Infeld theory the inversion of Eq. (2.13) is possible; we restrict ourselves to Lagrangians such that the passage to the canonical formalism is possible.

One remark should be made concerning the formalism introduced. The assumption of Born and Infeld,[2] of Plebanski,[3] and of the present authors is that $f^{\alpha\beta}$ is the physically significant electromagnetic field tensor, while $p^{\alpha\beta}$ is a tensor with no direct physical meaning. While the various nonlinear field theories succeed in making $f^{\alpha\beta}$ well behaved, the tensor $p^{\alpha\beta}$ is, in general, divergent at the location of point sources. In fact, this is unavoidable; δ-function sources continue to play a part in these theories, and the tensor $p^{\alpha\beta}$ acts as a "buffer" between the singular sources and the field tensor, "absorbing" the singularities of the sources and allowing the field tensor to be well behaved.

B. Einstein–(Nonlinear) Maxwell Theory

Throughout Sec. 2A, care has been taken to express everything in a Lorentz-covariant way. In order to generalize the equations to the general-relativistic level two changes only are needed. First of all, the equations must be modified so that they become generally covariant; secondly, we must add the action of the gravitational field to the action of Eq. (2.7). Thus we replace every equation of Sec. 2A by a general-relativistic counterpart, for example,

$$f_{\mu\nu} = 2A_{[\mu,\nu]}, \quad (2.1G)$$

where the general relativistic equations are identical to their special relativistic counterparts with the following exceptions:

$${}^*f^{\alpha\beta} \equiv \frac{i}{2(-g)^{\frac{1}{2}}}\frac{\epsilon^{\alpha\beta\gamma\delta}}{}f_{\gamma\delta}, \quad (2.3G)$$

$$((-g)^{\frac{1}{2}}\,{}^*f^{\alpha\beta})_{,\beta} = 0, \quad (2.8aG)$$

$$2\left((-g)^{\frac{1}{2}}\frac{\partial L(F, G^2)}{\partial f_{\alpha\beta}}\right)_{,\beta} = 4\pi\sum_{a=1}^{N} e_a \int_{-\infty}^{+\infty} \delta_4(x^\alpha - a^\alpha)\, da^\alpha, \quad (2.8bG)$$

$$((-g)^{\frac{1}{2}}p^{\alpha\beta})_{,\beta} = 4\pi\sum_{a=1}^{N} e_a \int_{-\infty}^{+\infty} \delta_4(x^\alpha - a^\alpha)\, da^\alpha, \quad (2.17aG)$$

$$\left[(-g)^{\frac{1}{2}}\left(\frac{\partial H}{\partial P}{}^*p^{\alpha\beta} + \frac{\partial H}{\partial Q}p^{\alpha\beta}\right)\right]_{,\beta} = 0. \quad (2.17bG)$$

Consistent with these equations is the modified action, which now includes a contribution from the gravitational field and is given by

$$W = -\sum_{a=1}^{N} m_a c\int_{\sigma_1}^{\sigma_2} dS_a + \sum_{a=1}^{N}\frac{e_a}{c}\int_{\sigma_1}^{\sigma_2} A_\alpha(a)\, da^\alpha - \frac{1}{4\pi c}\int_{\sigma_1}^{\sigma_2}(-g)^{\frac{1}{2}}L(F, G^2)\, d^4x + \frac{c^3}{16\pi k}\int_{\sigma_1}^{\sigma_2} R(-g)^{\frac{1}{2}}\, d^4X, \quad (2.7G)$$

where k is the gravitational constant, and $R = R_{\alpha\beta}g^{\alpha\beta}$ is the scalar curvature. The basic differential equations (using the canonical formalism) are thus Eqs. (2.17G) and the gravitational field equations,

$$G^{\alpha\beta} = -\frac{8\pi k}{c^4}\left[(-g)^{\frac{1}{2}}\sum_{a=1}^{N} m_a c^2\int_{\sigma_1}^{\sigma_2}\delta_4(x^\alpha - a^\alpha)\frac{da_a^\alpha}{dS_a}\frac{da_a^\beta}{dS_a}dS_a - \frac{1}{4\pi}\left(g^{\alpha\beta}L - \frac{\partial L}{\partial F}f^{\alpha\sigma}f_\sigma^\beta - \frac{\partial L}{\partial G}{}^*f^{\alpha\sigma}f_\sigma^\beta\right)\right], \quad (2.18G)$$

where $G^{\alpha\beta}$ is the Einstein tensor. These latter equations can of course be derived by setting $\delta W/\delta g_{\alpha\beta} = 0$.

3. A STATIC, SPHERICALLY SYMMETRIC SOLUTION

In looking for an SSS solution it would be natural to work in spherical polar coordinates r, θ, ϕ, and some time coordinate t. However, such coordinates would be singular on the world line of the point source, $r = 0$, and this world line is of importance to us. Thus, although many of our results will eventually be transformed to such coordinates, we begin with a different coordinate system, well behaved on the world line of the source.

It is well known[5] that a static, spherically symmetric metric can always be put in the form

$$dS^2 = e^\nu\, dt^2 - \sum_{a,b=1}^{3}\left[\delta_{ab} - (1 - e^\lambda)\frac{\xi^a}{r}\frac{\xi^b}{r}\right]d\xi^a\, d\xi^b, \quad (3.1)$$

where $r^2 \equiv \xi^{1^2} + \xi^{2^2} + \xi^{3^2}$ and ν and λ depend only on r. Thus we have

$$g \equiv |g_{\mu\nu}| = -e^{\nu+\lambda}. \quad (3.2)$$

[5] P. G. Bergmann, *Introduction to the Theory of Relativity* (Prentice-Hall, Inc., Englewood Cliffs, N.J., 1942).

We now assume that $\lim_{r\to 0} e^{\lambda}$ and $\lim_{r\to 0} e^{\nu}$ exist, and that

$$\lim_{r\to 0} e^{\lambda} = 1, \tag{3.3}$$

which makes our coordinate system well behaved on the world line $r = 0$.

We work in the Lagrangian formalism, and we must therefore solve Eqs. (2.8G) for the electromagnetic field tensor. It is clear from the form of the line element [Eq. (3.1)] that the three space coordinates are on equal footing; thus our spherically symmetric and static vector potential must be of the form

$$\bar{A}_{\mu} = (\bar{\phi}(r), \psi(r), \psi(r), \psi(r)).$$

A gauge can always be found such that, in fact,

$$A_{\mu} = (\phi(r), 0, 0, 0). \tag{3.4}$$

We automatically satisfy Eqs. (2.8aG) by deriving $f_{\alpha\beta}$ from A_{β} according to Eq. (2.1G), and consequently the only nonvanishing components of $f_{\alpha\beta}$ are

$$f_{0a} = \phi_{,r}\frac{\xi^a}{r}. \tag{3.5}$$

We can calculate the invariant and pseudoinvariant determined by Eq. (3.5), and we find

$$F = \tfrac{1}{2}f_{0a}f^{0a}, \quad G = 0, \tag{3.6}$$

and consequently Eq. (2.10G) and Eq. (2.6) implies that

$$p^{\alpha\beta} = \frac{\partial L}{\partial F} f^{\alpha\beta}. \tag{3.7}$$

The point source to be used in Eqs. (2.8bG) has the world line

$$a^{\alpha} = x^0\delta_0^{\alpha} \tag{3.8}$$

in our coordinates. Therefore, Eqs. (2.8bG) can be written in the form

$$\left((-g)^{\frac{1}{2}}\frac{\partial L}{\partial F} f^{ab}\right)_{,b} + \left((-g)^{\frac{1}{2}}\frac{\partial L}{\partial F} f^{a0}\right)_{,0} = 0, \tag{3.9}$$

$$\left((-g)^{\frac{1}{2}}\frac{\partial L}{\partial F} f^{0a}\right)_{,a} = 4\pi e\delta_3(\xi^a). \tag{3.10}$$

The first equation, (3.9), is automatically satisfied, since $f^{ab} = 0$ and f^{a0} is time-independent. As for the second equation, (3.10), it is obviously satisfied by

$$(-g)^{\frac{1}{2}}\frac{\partial L}{\partial F} f^{0a} = \frac{e}{r^2}\frac{\xi^a}{r},$$

and from this we find the covariant components of the field tensor which are nonvanishing to be

$$f_{0a} = -e^{(\nu+\lambda)/2}\frac{e\xi^a}{r^3}\Big/\frac{\partial L}{\partial F}(F, 0). \tag{3.11}$$

This expression can be put into a more convenient form. It follows from Eq. (2.13) and from $G = 0$ that we must have $Q = 0$. Then, from Eq. (2.16), follows

$$f^{\alpha\beta} = \frac{\partial H}{\partial P}(P, 0)p^{\alpha\beta}. \tag{3.12}$$

A comparison of Eqs. (3.7) and (3.12) yields

$$\frac{\partial H}{\partial P}(P, 0) = 1\Big/\frac{\partial L}{\partial P}(F, 0) \tag{3.13}$$

and thus

$$f_{0a} = -\frac{\partial H}{\partial P}(P, 0)e^{(\nu+\lambda)/2}\frac{e\xi^a}{r^3}. \tag{3.14}$$

[Comparison with Eq. (3.5) allows an identification of the potential function $\phi(r)$ in terms of H, ν, and λ.] Thus the generalized Maxwell's equation have been satisfied. The behavior of the $p^{\alpha\beta}$ field,

$$p^{\alpha\beta} = \delta_0^{\alpha}\delta_a^{\beta}e^{(-\nu-\lambda)/2}\frac{e}{r^2}\frac{\xi^a}{r}, \tag{3.15}$$

at $r = 0$ is obviously singular; however, that of $f^{\alpha\beta}$ depends on $\partial H(P, 0)/\partial P$, and that is as yet unspecified. It shall be specified in such a way as to make $f^{\alpha\beta}$ well behaved at $r = 0$.

It is convenient to approach the question by considering Eq. (2.9G), the equation for the Lorentz force. Putting $m_a = 0$ in this equation, consistent with our assumption that the point source has no mass, and using the world line for the point source given by Eq. (3.8) give us

$$f_{0a}(0) = 0. \tag{3.16}$$

This is a condition on $\partial H(P, 0)/\partial P$ of the form

$$\lim_{r\to 0} e^{(\nu+\lambda)/2}\frac{\xi^a}{r^3}\frac{\partial H}{\partial P}(P, 0) = 0, \tag{3.17}$$

which, in view of the assumptions already made about $\nu(r)$ and $\lambda(r)$, reduces to

$$\lim_{r\to 0}\frac{\xi^a}{r^3}\frac{\partial H}{\partial P}(P, 0) = 0. \tag{3.18}$$

We now assume that the Hamiltonian for our theory is such that Eq. (3.18) is satisfied; this assures us that $f^{\alpha\beta}$ is continuous in the neighborhood of the charge and also that the Lorentz force equation is satisfied there.

It remains to solve Eqs. (2.17cG), the Einstein equations, for the functions $\nu(r)$ and $\lambda(r)$. It is a

lengthy but straightforward calculation to obtain $G^{\alpha\beta}$ and $T^{\alpha\beta}$ from $g_{\alpha\beta}$ and $f_{\alpha\beta}$. Using these results in Eqs. (2.17cG) gives us the following nontrivial equations:

$$e^{-\lambda}\left(\frac{1}{r^2}-\frac{\lambda'}{r}\right)-\frac{1}{r^2}=\frac{2k}{c^4}H(P,0) \tag{3.19}$$

and

$$\begin{aligned}&-\left(\frac{\nu'}{r}+\frac{1-e^{\lambda}}{r^2}\right)\frac{\xi^a\xi^b}{r^2}\\&\quad+\left(\frac{\nu''}{2}+\frac{\nu'(\nu'-\lambda')}{4}+\frac{\nu'-\lambda'}{2r}\right)\left(\frac{\xi^a\xi^b}{r^2}-\delta_{ab}\right)e^{-\lambda}\\&=\frac{2k}{c^4}L(F,0)\left(\delta_{ab}-\frac{\xi^a\xi^b}{r^2}\right)\\&\quad+\frac{2k}{c^4}\left[L-\frac{\partial L}{\partial F}f^{0a}f_{0a}\right]e^{\lambda}\frac{\xi^a\xi^b}{r^2}.\end{aligned} \tag{3.20}$$

We next eliminate $\partial L/\partial F$ from the last term of this equation by means of the relationship

$$2F\frac{\partial L}{\partial F}=H+L, \tag{3.21}$$

which can be derived from Eqs. (2.11) and (3.7). Using $F=\frac{1}{2}f^{0a}f_{0a}$ and matching coefficients in Eq. (3.20) give us

$$\frac{2k}{c^4}L(F,0)=\left[\frac{\nu''}{2}+\frac{\nu'}{4}(\nu'-\lambda')+\frac{1}{2r}(\nu'-\lambda')\right]e^{-\lambda} \tag{3.22}$$

and

$$\frac{2k}{c^4}H(P,0)=e^{-\lambda}\left(\frac{\nu'}{r}+\frac{1}{r^2}\right)-\frac{1}{r^2}. \tag{3.23}$$

We are now concerned with just three equations, Eqs. (3.19), (3.22), and (3.23). Combining Eqs. (3.19) and (3.23) yields $\lambda'+\nu'=0$, and so we have $\lambda+\nu=b$, an arbitrary constant. It can be shown that $b\neq 0$ will prevent the metric from being asymptotically Minkowskian, so we assume

$$\lambda+\nu=0. \tag{3.24}$$

We have reduced our problem to solving Eqs. (3.19) and (3.22) with $\lambda=-\nu$. But we note that there is a relation

$$2P\frac{\partial H}{\partial P}(P,0)=H+L, \tag{3.25}$$

analogous to Eq. (3.21), and, since

$$P=-e^2/2r^4,$$

it follows that $(r^2H)'=-2rL$ is identically satisfied here. If we calculate $(r^2H)'$ from Eq. (3.19) and use Eq. (3.25), we obtain Eq. (3.22). Thus we have only one independent equation, Eq. (3.19), and it is solved by

$$e^{-\lambda}=1+\frac{d}{r}+\frac{2k}{c^4}\frac{1}{r}\int_0^r t^2H(t)\,dt, \tag{3.26}$$

where d is an arbitrary constant. By comparison with the Schwarzschild solution we see that d is proportional to the mass of the point source, which we are assuming to be zero. Thus we have

$$e^{-\lambda}=1+\frac{2k}{c^4}\frac{1}{r}\int_0^r t^2H(t)\,dt. \tag{3.27}$$

We have accumulated several conditions on the behavior of H at $r=0$. First, our coordinates are valid only if

$$\lim_{r\to 0}e^{\lambda}=1,\quad \lim_{r\to 0}e^{\nu}\text{ exists.} \tag{3.28}$$

Secondly, the Lorentz force equation led us to demand that

$$\lim_{r\to 0}\frac{\partial H(P,0)}{\partial P}\frac{\xi^a}{r^3}=0. \tag{3.29}$$

Finally, the integral

$$\int_0^r t^2H(t)\,dt \tag{3.30}$$

in Eq. (3.27) must, of course, exist. No attempt has been made to find necessary and sufficient conditions on $H(P,0)$ in order to satisfy Eqs. (3.28) and (3.29). An example of a sufficiency condition is the assumption that

$$H(P,0)=\sum_{n=0}^{\infty}\frac{a_n}{P^n},\quad P>P_0, \tag{3.31}$$

and that this expansion is term-by-term differentiable and integrable.

It remains to consider our solution as $r\to\infty$. It is to be expected, in particular, that the metric tensor should be asymptotically Minkowskian, since the electromagnetic theory is asymptotically linear, but it is of interest to see the manner of the approach. Since we are no longer interested in the point $r=0$, it is now permissable (and very convenient) to transform to a generalization of spherical coordinates. Thus we do the coordinate transformation

$$\begin{aligned}\xi^1&=r\sin\theta\cos\phi,\\ \xi^2&=r\sin\theta\sin\phi,\\ \xi^3&=r\cos\theta,\\ t&=t,\end{aligned} \tag{3.32}$$

and obtain

$$dS^2=e^{-\lambda}\,dt^2-e^{\lambda}\,dr^2-r^2(d\theta^2+\sin^2\theta\,d\phi^2), \tag{3.33}$$

where $\lambda(r)$ is given, as before, by Eq. (3.27), while

$$f_{\alpha\beta} = -\frac{e}{r^2}\frac{\partial H(P,0)}{\partial P} 2\delta^{[0}_{\alpha}\delta^{r]}_{\beta}. \tag{3.34}$$

In order to examine the behavior of $g_{\alpha\beta}$ and $f_{\alpha\beta}$ for large r, we must make some assumption on the behavior of $H(P, 0)$ for large r consistent with the condition that for weak fields (meaning large r in this problem) the theory approach the linear theory. Since, in the linear theory $H = P$, we assume

$$H = P + \sum_{n=2}^{\infty} b_n P^n, \quad P < P_0', \tag{3.35}$$

and that this expansion is term-by-term differentiable. It then follows that, for large r,

$$f_{\alpha\beta} = -\frac{e}{r^2} + O(r^{-6}) \tag{3.36}$$

and

$$e^{-\lambda} = 1 - \frac{2k}{c^2}\frac{M}{r} + \frac{ke^2}{c^4}\frac{1}{r^2} + (r^{-6}), \tag{3.37}$$

where

$$M \equiv -\int_0^{\infty} t^2 H(t)\, dt. \tag{3.38}$$

Thus, our solution approaches the Riesner–Nordstrom solution[5] for large r with the M of Eq. (3.38) identified as mass. This mass is of course defined purely in terms of the long-range gravitational effects associated with the point charge; the mass of the point source has been consistently set equal to zero. The mass M can also be put into the form

$$M = (2e/3c^2)\phi(0) \tag{3.39}$$

which relates the asymptotically defined mass with the value of the electromagnetic potential function at $r = 0$. This latter result follows if the potential is normalized to be zero at infinity.

4. CONCLUSION

We summarize here the results obtained, along with the assumptions made. We consider the Einstein–(nonlinear) Maxwell equations, where the form of the nonlinear Maxwell theory is determined by the Hamiltonian $H(P, Q)$ or, alternatively, by the Lagrangian $L(F, G)$. We assume that, for $Q = 0$, $H(P, Q)$ is expandable in positive powers of P for $P < P_0$ and in negative powers of P for $P > P_0$ and that these expansions are term-by-term differentiable and integrable. We also assume that the integral

$$\int_0^r H(P, 0) r^2\, dr$$

(where $p = -e^2/2r^4$) is defined for all r including $r = \infty$.

We then show that there exists a static, spherically symmetric solution of the Einstein–(nonlinear) Maxwell equations with the following properties:

(1) Both the electromagnetic and the metric tensors are well behaved at $r = 0$;

(2) the metric is, asymptotically, the Riesner–Nordstrom metric with a mass identification

$$M = -\int_0^{\infty} t^2 H(-e^2/2t^2, 0)\, dt;$$

(3) the Lorentz equation is satisfied at $r = 0$.

The above solution corresponds to a source which has a δ-function charge distribution at $r = 0$, but vanishing mass. It should be emphasized that the assumptions made are certainly stronger than necessary.

A final comment is that certain difficulties of the Born–Infeld nonlinear electrodynamics are in no way eliminated in this work. In particular, the general relativistic equations have characteristic surfaces corresponding to propagation velocities exceeding the speed of light, just as did the special relativistic theories.[3]

ACKNOWLEDGMENT

The authors are indebted to Professor J. Plebanski for conceiving and initiating this problem.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

General Form of the Einstein Equations for a Bianchi Type IX Universe*

MICHAEL P. RYAN, JR.†
Department of Physics and Astronomy, University of Maryland, College Park, Maryland

(Received 24 February 1969)

The Einstein equations for a general Bianchi type IX universe are presented in a form suitable for numerical solution. As an example, the complete equations for a cosmology with a pure fluid stress tensor $T_{\mu\nu} = \epsilon u_\mu u_\nu + p(g_{\mu\nu} + u_\mu u_\nu)$ are also given.

I. INTRODUCTION

In recent years there has been some interest shown in models of the universe that are more complicated than the highly symmetric Friedmann cosmologies.[1] The first step in investigating less symmetric universes has been to consider universes which still have a global time coordinate and homogeneous space sections at any one time, but which no longer obey the requirement of isotropy. The study of such universes naturally leads to investigation of homogeneous three-spaces, the study of which goes back to Bianchi,[2] who divided them into nine classes according to the groups of motions under which the space is invariant.

Until recently there has been little interest in these anisotropic universes as possible cosmologies because the meager cosmological data available have always been explicable in terms of the Friedmann models or models with similar high symmetry. A few years ago there was a resurgence of interest in these more general models spurred by Gödel[3] and they are discussed by Taub[4] and Heckmann and Schücking.[1] In the past five years, several works have appeared using anisotropic universes to consider such problems as helium production and magnetic fields in the universe.[5–8] The geometrical questions for these universes were long ago treated in great detail by Cartan.[9]

Quite recently, the discovery of the 3°K microwave background[10] and its interpretation as a cosmological phenomenon[11] have led to increased interest in these universes as physical entities. The discovery by Partridge and Wilkinson[12] of the remarkable isotropy of this radiation has provided cosmology with its first extremely accurate datum. Investigation of the causes of this isotropy has led Misner[13] to use some fruitful mathematical techniques in a Bianchi type I universe that promise to be useful in studying the evolution of universes in general. In a more recent paper Misner[14] has used these same techniques in a study of a special case of a type IX universe, a generalization of the Friedmann $k = +1$ cosmology. These two works lead naturally to the present study, by means of the same techniques of a more general type IX universe, and to the study of type V cosmologies, generalizations of the Friedmann $k = -1$ universe.[15]

Universes of types V and IX have an important advantage over type I in that G_{0i} need not be zero for these cases (though it may be[14]) and hence T^{0i}, which is directly related to the local fluid velocity, need not be zero. The existence of a nonzero local fluid velocity can lead to the existence of rotation as defined by the existence of a nonzero angular-velocity tensor as defined by Ehlers[16]:

$$\Omega_{\mu\nu} = U_{[\mu;\nu]} + U_{[\mu;\alpha}U^\alpha U_{\nu]},$$

where U_μ is the fluid velocity.

In this paper we intend to present, in the form of a progress report, the Einstein equations for a type IX cosmology with a pure fluid source. Estabrook, Wahlquist, and Behr[17,18] and Shepley[19] have studied the equations for this type of cosmology in different

* Supported in part by NASA Grant NGR-21-002-010. This work is part of a Ph.D. thesis to be submitted to the University of Maryland.

† NSF Predoctoral Trainee.

[1] See O. Heckmann and E. Schücking, in *Gravitation: An Introduction to Current Research*, L. Witten, Ed. (John Wiley & Sons, Inc., New York, 1962), Chap. 11.

[2] I. Bianchi, Mem. Soc. Ital. Sci., Ser. IIIa, 11 (1897).

[3] K. Gödel, Proc. Intern. Congr. Math. **1**, 175 (1950).

[4] A. Taub, Ann. Math. **53**, 472 (1951).

[5] Ya. B. Zel'dovich, Astron. Zh. **41**, 873 (1964) [Sov. Astron.—AJ **8**, 700 (1965)].

[6] Ya. B. Zel'dovich, Zh. Eksp. Teor. Fiz. **48**, 986 (1965) [Sov. Phys.—JETP **21**, 656 (1965)].

[7] K. S. Thorne, Astrophys. J. **148**, 51 (1967).

[8] S. Hawking and R. Tayler, Nature **209**, 1278 (1966).

[9] E. Cartan, *Lecons sur la geometrie des espaces de Riemann* (Gauthier-Villars, Paris, 1951).

[10] A. Penzias and R. Wilson, Astrophys. J. **142**, 419 (1965).

[11] R. Dicke, P. Peebles, P. Roll, and D. Wilkinson, Astrophys. J. **142**, 414 (1965).

[12] R. Partridge and D. Wilkinson, Phys. Rev. Letters **18**, 557 (1967).

[13] C. Misner, Astrophys. J. **151**, 431 (1968).

[14] C. Misner, Phys. Rev. Letters **22**, 1071 (1969).

[15] For a discussion of a type V universe, see R. Matzner, Astrophys. J. (to be published).

[16] J. Ehlers, Akad. Wiss. Lit. (Mainz) Abhandl. Math. Nat. Kl. **11** (1961).

[17] C. Behr, Astron. Abhandl. Hbg. Sternwarte **7**, 249 (1965).

[18] F. Estabrook, H. Wahlquist, and C. Behr, J. Math. Phys. **9**, 497 (1968).

[19] L. Shepley, Dissertation, Princeton, 1965.

tetrad frames and with different goals. We present our work as exhibiting a set of equations in a manner which lends itself naturally to machine calculation. It is hoped that the introduction of rotation into the solution will provide some interesting results that do not appear in nonrotating cosmologies.[20]

II. A MODEL OF THE UNIVERSE

We shall take as a metric to describe a type IX universe

$$ds^2 = -dt^2 + g_{ij}(t)\sigma_i\sigma_j, \tag{1}$$

where the σ_i are a set of homogeneous differential one-forms on the three-sphere. If we let the three-sphere be described as $S^3 = \{x, y, z, w \mid x^2 + y^2 + z^2 + w^2 = 1\}$, then the forms can be written

$$\begin{aligned} \sigma_x &= x\,dw - w\,dx - z\,dy + y\,dz, \\ \sigma_y &= y\,dw + z\,dx - w\,dy - x\,dz, \\ \sigma_z &= z\,dw - y\,dx + x\,dy - w\,dz. \end{aligned} \tag{2}$$

These forms are discussed by Misner,[21] who gives a proof that they are indeed invariant under motions on S^3. Since the tangent vectors dual to these forms, when considered as the infinitesimal generators of a Lie group, have structure constants $C^i_{jk} = \epsilon_{ijk}$, this metric indeed describes a type IX universe.[1]

Once we have the above metric, we need a stress–energy tensor to act as a source for the Einstein equations. To indicate how these Einstein equations and supplementary conditions such as $T^{\mu\nu}{}_{;\nu} = 0$ combine to give a set of differential and algebraic equations for all relevant quantities, we will take as an exemplary stress–energy tensor that of a perfect fluid

$$T^{\mu\nu} = \epsilon U^\mu U^\nu + p(g^{\mu\nu} + U^\mu U^\nu), \tag{3}$$

where ϵ and p are the usual energy density and pressure, respectively.

Several other stress–energy tensors are also of interest; those most carefully investigated at present are those of collisionless radiation and viscous radiation. Misner,[13] Misner and Matzner,[22] Doroshkevich *et al.*,[23] and Stewart[24] have studied these types of radiation in type I universes and are continuing to investigate them. In universes with curved space sections these forms of radiation are more difficult to describe and will not be considered in this paper.

[20] While this paper was being typed, a preprint by S. Hawking (Cambridge) considering this subject was received. This has since been published in Monthly Notices Roy. Astron. Soc. (London) **142**, 129 (1969).

[21] C. Misner, J. Math. Phys. **4**, 924 (1963).

[22] C. Misner and R. Matzner (to be published).

[23] A. Doroshkevich, Ya. B. Zel'dovich, and I. Novikov. Zh. Eksp. Teor. Fiz. Pis. Red. **5**, 119 (1967) [JETP Letters **5**, 96 (1967)].

[24] J. Stewart, Astrophys. Letters **2**, 133 (1968).

Since the G_{0i} need not be zero in a type IX universe, we cannot assume that $U^\mu = \delta^\mu{}_0$, but must in general let $U^\mu = (\gamma, U^1, U^2, U^3)$, where $U^\mu U_\mu = -1$ determines γ. The three new independent quantities $U^i(t)$ will be determined by the three G_{0i} Einstein equations. In the general case where no restrictions are placed on the U^i we should see rotation as indicated by the existence of a nonvanishing scalar of rotation Ω, where $\Omega^2 = \frac{1}{2}\Omega_{\mu\nu}\Omega^{\mu\nu}$, with $\Omega_{\mu\nu}$ as defined above. Since no explicit solutions for type IX universes with expansion, rotation, and shear have been presented, one should expect that such solutions would predict observable effects which do not appear in the simpler solutions. It is especially hoped that these solutions will provide more arguments in support of the observed isotropy of the 3°K black-body radiation.

III. THE EINSTEIN EQUATIONS

We begin by writing the $g_{ij}(t)$ in the metric of Sec. II as $R^2(t)(B^{\mathrm{T}}B)_{ij}$. Since the 3×3 matrix B_{ij} appears in the metric components only in the combination $(B^{\mathrm{T}}B)_{ij}$ and since only these components determine the physical behavior of the system, there is some freedom in the choice of $B_{ij}(t)$. It is most convenient to make B definite by requiring that $\dot{B}B^{-1}$ ($\dot{B} \equiv dB/dt$) be a symmetric matrix, that is,

$$(\dot{B}B^{-1})^{\mathrm{T}} = \dot{B}B^{-1}. \tag{4}$$

With this choice we can proceed to define[14] an orthonormal frame

$$\omega^0 = dt, \quad \omega^i = RB_{ij}\sigma_j \tag{5}$$

and write the metric as

$$ds^2 = \eta_{\mu\nu}\omega^\mu\omega^\nu, \tag{6}$$

where $\eta_{\mu\nu}$ is a Minkowski metric of signature $(- + + +)$. We can now calculate the Einstein equations for our metric in this frame. The details of this calculation are given in Appendix A. The results are (in units with $G = c = 1$)

$$8\pi T_{00} = 3(\dot{R}/R)^2 - \tfrac{1}{2}R^{-6}\,\mathrm{Tr}\,[(S)^2] - \tfrac{1}{4}R^{-2}\,\mathrm{Tr}\,[(B^{\mathrm{T}}B)^2 - (B^{\mathrm{T}}B)^{-1}], \tag{7a}$$

$$8\pi T_{0i} = \tfrac{1}{2}R^{-4}[S, (B^{\mathrm{T}}B)]_{jk}\epsilon_{ijk}, \tag{7b}$$

$$8\pi(T_{ij} - \tfrac{1}{3}\delta_{ij}T^k{}_k) = \{R^{-3}\dot{S} + R^{-2}[(B^{\mathrm{T}}B)^2 + (B^{\mathrm{T}}B)^{-1}]\}_{ij} - \tfrac{1}{3}\delta_{ij}R^{-2}\mathrm{Tr}\,[(B^{\mathrm{T}}B)^2 + (B^{\mathrm{T}}B)^{-1}], \tag{7c}$$

$$\tfrac{8}{3}\pi T^k{}_k = -2\ddot{R}/R - (\dot{R}/R)^2 - \tfrac{1}{2}R^{-6}\,\mathrm{Tr}\,[(S)^2] - \tfrac{1}{12}R^{-2}\,\mathrm{Tr}\,[(B^{\mathrm{T}}B)^2 - 2(B^{\mathrm{T}}B)^{-1}], \tag{7d}$$

where $S = (\dot{B}B^{-1})R^3$, $[A, B]$ is the commutator of the matrices A and B, and ϵ_{ijk} is the totally antisymmetric symbol with $\epsilon_{1\,2\,3} = +1$.

IV. THE EQUATIONS OF MOTION FOR THE MODEL

With the above metric and stress tensor describing our model of the universe, the quantities whose development we would like to follow are R, B_{ij}, ϵ, p, and U_μ. We need to organize the Einstein equations in a manner that will facilitate numerical computation of relevant quantities. This organization is much simpler if we introduce, following Landau and Lifshitz[25] and Misner and Sharp,[26] the baryon number density n and the specific entropy s as variables to replace p and ϵ. From thermodynamic considerations we can specify for our fluid an equation of state $\epsilon = \epsilon(n, s)$ and deduce p by means of the relation $p = n(\partial\epsilon/\partial n)_s - \epsilon$. With these substitutions we present such an organization of the Einstein equations. To avoid repetition, once in a derivation and a second time in a list, the derivation of this set of equations is given after the list.

The *fundamental variables* entering the scheme are R, B_{ij}, S_{ij} (defined above), and n (s will be shown to be constant for this problem). We may simplify the writing of the differential equations by defining the following *auxiliary quantities*:

$$8\pi\phi_i = \tfrac{1}{2}R^{-4}[S, (B^{\mathrm{T}}B)]_{jk}\epsilon_{ijk}, \tag{8a}$$

$$\phi^2 = \phi_i\phi_i. \tag{8b}$$

The *dynamic equations* or time-step differential equations allow one in a numerical integration scheme to update the values of the fundamental variables. They are

$$(\dot{R}/R)^2 = \tfrac{1}{2}R^{-6}\,\mathrm{Tr}\,[(S)^2] - (\tfrac{1}{4})R^{-2}\,\mathrm{Tr}\,[(B^{\mathrm{T}}B)^2 - (B^{\mathrm{T}}B)^{-1}] \tag{9a}$$

$$-8\pi(\tfrac{1}{2}\{(\epsilon + p) + [(\epsilon + p)^2 + 4\phi^2]^{\frac{1}{2}}\} - p),$$

$$\dot{B}_{ij} = (SB)_{ij}R^{-3}, \tag{9b}$$

$$\dot{S}_{ij} = R[(B^{\mathrm{T}}B) + (B^{\mathrm{T}}B)^{-1}]_{ij} - \tfrac{1}{3}\delta_{ij}R\,\mathrm{Tr}\,[(B^{\mathrm{T}}B) + (B^{\mathrm{T}}B)^{-1}] - \frac{8\pi(\phi_i\phi_j - \frac{1}{3}\delta_{ij}\phi^2)}{\{\frac{1}{2}[(\epsilon + p) + ((\epsilon + p)^2 + 4\phi^2)^{\frac{1}{2}}]\}}, \tag{9c}$$

$$n = \nu/\gamma R^3, \tag{9d}$$

where ν is a constant.

Equations (9a)–(9c) are obtained by inserting $T^{\mu\nu} = \epsilon U^\mu U^\nu + p(\eta^{\mu\nu} + U^\mu U^\nu)$ into the Einstein equations and using $T^{0i} = (\epsilon + p)\gamma U^i = \phi_i$ to eliminate U^i from the resulting relations. Equation (9d) is a consequence of the fact that $T^{\mu\nu}{}_{;\nu} = 0$. It can be shown[26] that $U_\mu T^{\mu\nu}{}_{;\nu} = 0$ implies the two equations

$$(nU^\mu)_{;\mu} = 0, \tag{10a}$$

$$U^\mu s_{,\mu} = 0. \tag{10b}$$

Because s can only depend on time, (10b) implies $\dot{s} = 0$ or that; as stated above, s is a constant. Thus $\epsilon = \epsilon(n)$ and $p = n(d\epsilon/dn) - \epsilon$. If we compute the left-hand side of (10a) in our orthonormal frame by means of the methods given in Appendix B, we find that the equation becomes

$$\frac{3\dot{R}}{R} + \frac{\dot{\gamma}}{\gamma} + \frac{\dot{n}}{n} = 0, \tag{11}$$

which has Eq. (9d) as its solution.

Note that (9d) and the equation

$$\gamma = (\tfrac{1}{2}\{1 + [1 - 4\phi^2/(\epsilon + p)^2]^{\frac{1}{2}}\})^{\frac{1}{2}}$$

form a set of two algebraic equations in the two unknowns γ and n at any one time. Because these are algebraic and not differential equations, it will be necessary to solve them explicitly or iteratively for γ or n in terms of R, B, and S in order to use updated values of these variables to obtain updated γ and n.

In order to check the accuracy of a numerical integration scheme for these equations, we would like to have several quantities which may be obtained both by means of equations giving them at any one stage of the solution and by numerical differentiation between two successive stages. Two such checks are equations for $\ddot{R}$ and $\dot{U}_i$ obtained from the $T^k{}_k$ equation and from the space part of the Euler equation

$$U_{\mu;\nu}U^\nu = -[1/(\epsilon + p)](\delta^\nu{}_\mu + U_\mu U^\nu)p_{,\nu},$$

respectively ($U_{\mu;\nu}$ is given in Appendix B). These equations are

$$\dot{U}_i = \frac{\dot{p}}{\epsilon + p}U_i - \frac{\dot{R}}{R}U_i - R^{-3}S_{ij}U_j - R^{-1}\gamma^{-1}(B^{\mathrm{T}}B)_{jl}U_jU_k\epsilon_{ikl}, \tag{12a}$$

$$\ddot{R} = -\frac{1}{2}\frac{(\dot{R})^2}{R} - \tfrac{1}{4}R^{-5}\,\mathrm{Tr}\,[(S)^2] - \tfrac{1}{24}R^{-1}\,\mathrm{Tr}\,[(B^{\mathrm{T}}B)^2 - 2(B^{\mathrm{T}}B)^{-1}] - \frac{8\pi}{3}R\left(\frac{\phi^2}{(\epsilon + p)\gamma^2} + 3p\right). \tag{12b}$$

Given the fundamental variables as functions of time, we can calculate the following physically important

[25] L. Landau and E. Lifshitz, *Fluid Mechanics* (Addison-Wesley Publ. Co., Inc., Reading, Mass., 1959), Chap. XV.

[26] C. Misner and D. Sharp, Phys. Rev. **136B**, 571 (1964).

quantities:

$$g_{ij} = R^2(B^{\mathrm{T}}B)_{ij},$$
$$\gamma = (\tfrac{1}{2}\{1 + [1 + 4\phi^2/(\epsilon + p)^2]^{\frac{1}{2}}\})^{\frac{1}{2}},$$
$$\epsilon = \epsilon(n),$$
$$p = n\frac{d\epsilon}{dn} - \epsilon,$$
$$U_i = \phi_i/\gamma(\epsilon + p),$$
$$\theta = \dot{\gamma} + 3(\dot{R}/R)\gamma,$$
$$\Omega_{0i} = \tfrac{1}{2}\{\dot{U}_i - [pU_i/(\epsilon + p)] - (\dot{R}/R)U_i - R^{-3}S_{ij}U^j\},$$
$$\Omega_{ij} = -\tfrac{1}{2}U_k R^{-1}(B^{\mathrm{T}}B)_{kl}\epsilon_{lij},$$
$$\Omega^2 = \tfrac{1}{2}\Omega_{\mu\nu}\Omega^{\mu\nu},$$
$$\Sigma_{00} = \dot{\gamma} + \{(\theta/3) - [\gamma\dot{p}/(\epsilon + p)]\}(\gamma^2 - 1),$$
$$\Sigma_{0i} = -\tfrac{1}{2}[(\dot{R}/R)U_i + R^{-3}S_{ij}U_j - \dot{U}_i + U_i[\dot{p}/(\epsilon + p)](1 - 2\gamma^2)] + \tfrac{1}{3}\theta\gamma U_i,$$
$$\Sigma_{ij} = -\tfrac{1}{3}\dot{\gamma}\delta_{ij} + \gamma R^{-3}S_{ij} + \tfrac{1}{2}R^{-1} \times [(B^{\mathrm{T}}B)_{il}\epsilon_{ljk} + (B^{\mathrm{T}}B)_{lj}\epsilon_{lik}]U^k - \frac{\gamma\dot{p}}{\epsilon + p}U_iU_j - \tfrac{1}{3}\theta U_iU_j,$$
$$\Sigma^2 = \tfrac{1}{2}\Sigma_{\mu\nu}\Sigma^{\mu\nu},$$

where $\Omega_{\mu\nu}$ is defined above, $\Sigma_{\mu\nu}$ is the tensor of shear defined by Ehlers,[16] and θ is the scalar of expansion also defined by Ehlers.

In a future paper we expect to present and discuss solutions of the above equations for a variety of initial conditions. With these solutions we can begin to investigate the observational consequences of rotation. We may hope that these consequences will include more detailed explanations for the isotropy of the 3°K blackbody radiation.

ACKNOWLEDGMENT

The author wishes to acknowledge the constant encouragement and guidance of Professor C. W. Misner throughout this work.

APPENDIX A

Instead of computing the Einstein equations directly in the orthonormal frame $\omega_i = RB_{ij}\sigma_j$, it is much simpler to define, following Misner,[13] a matrix β and a scalar α by

$$ds^2 = -dt^2 + e^{2\alpha}e^{2\beta}{}_{ij}\sigma_i\sigma_j$$

with $\det e^{\beta} = e^{\mathrm{Tr}\,\beta} = 1$ ($\mathrm{Tr}\,\beta = 0$), do the computation in the frame $\omega_i = e^{\alpha}e^{\beta}{}_{ij}\sigma_j$, and transform to the desired frame afterwards. Once we have made this choice, we can proceed in the same manner as Misner[13] with the addition of the general result

$$d\sigma_i = \tfrac{1}{2}\epsilon_{ijk}\sigma_j \wedge \sigma_k,$$

where d represents an exterior derivative on the forms σ_i. By requiring that this exterior derivative represent a torsionless, covariant derivative, we have

$$d\omega^{\mu} = -\omega^{\mu}{}_{\nu} \wedge \omega^{\nu}, \tag{A1a}$$
$$dg_{\mu\nu} = d\eta_{\mu\nu} = 0 = \omega_{\mu\nu} + \omega_{\nu\mu}. \tag{A1b}$$

From these we have

$$d\omega^0 = d(dt) = 0 = -\omega^0{}_i \wedge \omega^i, \tag{A2a}$$
$$d\omega^i = [\dot{\alpha}e^{\alpha}e^{\beta} + e^{\alpha}(\dot{e}^{\beta})]\sigma_j \wedge \omega^0 + \tfrac{1}{2}e^{\alpha}e^{\beta}{}_{ij}\epsilon_{jkl}\sigma_k \wedge \sigma_l. \tag{A2b}$$

Defining

$$\sigma = \tfrac{1}{2}[(e^{\beta})\cdot e^{-\beta} + e^{-\beta}(e^{\beta})\cdot]$$

and

$$\tau = \tfrac{1}{2}[(e^{\beta})\cdot e^{-\beta} - e^{-\beta}(e^{\beta})\cdot]$$

and using $\sigma_j = e^{-\alpha}e^{-\beta}{}_{ij}\omega^i$, for (A2b) we find

$$d\omega^i = \dot{\alpha}\omega^i \wedge \omega^0 + [\sigma + \tau]_{ij}\omega^j \wedge \omega^0 + \tfrac{1}{2}e^{-\alpha}e^{2\beta}{}_{ik}\epsilon_{kmn}\omega^m \wedge \omega^n. \tag{A3}$$

If we define Γ_{ijm} (antisymmetric in i and j) by

$$\Gamma_{ijm}\omega^m \wedge \omega^j = \tfrac{1}{2}e^{-\alpha}e^{2\beta}{}_{ik}\epsilon_{kmj}\omega^m \wedge \omega^j,$$

we find that

$$\Gamma_{ijm} = \tfrac{1}{2}e^{-\alpha}(e^{2\beta}{}_{ik}\epsilon_{kmj} + e^{2\beta}{}_{jk}\epsilon_{kim} - e^{2\beta}{}_{mk}\epsilon_{kji}) \tag{A4}$$

and $\omega_{ij} = \Gamma_{ijm}\omega^m + \tau_{ij}\omega^0$. The other nonzero $\omega^{\mu}{}_{\nu}$ are $\omega^0{}_i = (\dot{\alpha}\delta^i{}_j + \sigma_{ij})\omega_j$.

With these forms at hand we can obtain $R_{\mu\nu\alpha\beta}$ from the curvature forms

$$\theta^{\mu}{}_{\nu} = d\omega^{\mu}{}_{\nu} + \omega^{\mu}{}_{\alpha} \wedge \omega^{\alpha}{}_{\nu} \tag{A5}$$

and the expression $\theta_{\mu\nu} = \tfrac{1}{2}R_{\mu\nu\alpha\beta}\omega^{\alpha} \wedge \omega^{\beta}$. Inserting our values for $\omega^{\mu}{}_{\nu}$ above, we find

$$\begin{aligned}\theta_{01} &= -\theta^0{}_1 \\ &= -(\ddot{\alpha}\delta^1{}_j + \dot{\sigma}_{1j})\omega^0 \wedge \omega^j \\ &\quad + (\dot{\alpha}\delta^1{}_j + \sigma_{1j})(\dot{\alpha}\delta^j{}_k + \sigma_{jk})\omega^k \wedge \omega^0 \\ &\quad + (\dot{\alpha}\delta^1{}_j + \sigma_{1j})\tau_{jk}\omega^0 \wedge \omega^k - (\dot{\alpha}\delta^1{}_j + \sigma_{1j})\Gamma_{jkm}\omega^m \wedge \omega^k \\ &\quad - (\dot{\alpha}\delta^2{}_j + \sigma_{2j})\tau_{21}\omega^j \wedge \omega^0 - (\dot{\alpha}\delta^2{}_j + \sigma_{2j})\Gamma_{21m}\omega^j \wedge \omega^m \\ &\quad - (\dot{\alpha}\delta^3{}_j + \sigma_{3j})\tau_{31}\omega^j \wedge \omega^0 - (\dot{\alpha}\delta^3{}_j + \sigma_{3j})\Gamma_{31m}\omega^j \wedge \omega^m\end{aligned} \tag{A6}$$

(with similar expressions for θ_{02} and θ_{03}) and

$$\begin{aligned}\theta_{23} &= \theta^2{}_3 \\ &= -\Gamma_{23m}\omega^0 \wedge \omega^m + \Gamma_{23m}(\dot{\alpha}\delta^m{}_j + \sigma_{mj} + \tau_{mj})\omega^j \wedge \omega^0 \\ &\quad + \Gamma_{23m}\Gamma_{mjk}\omega^j \wedge \omega^k - \tau_{21}\Gamma_{13m}\omega^0 \wedge \omega^m \\ &\quad + \tau_{31}\Gamma_{21m}\omega^m \wedge \omega^0 + \Gamma_{21m}\Gamma_{13n}\omega^m \wedge \omega^n \\ &\quad + (\dot{\alpha}\delta^2{}_j + \sigma_{2j})(\dot{\alpha}\delta^3{}_k + \sigma_{3k})\omega^j \wedge \omega^k\end{aligned} \tag{A7}$$

(with similar expressions for θ_{13} and θ_{12}). Due to the antisymmetry of $\theta_{\mu\nu}$, these six quantities are sufficient to find $R_{\mu\nu\alpha\beta}$. We may now calculate $R_{\mu\nu} = R^{\alpha}{}_{\mu\alpha\nu}$ and $R = R_{\mu}{}^{\mu}$ by inspection. Inserting our expression for Γ_{ijk} from Eq. (A4), we find that

$$R_{00} = 3\ddot{\alpha} - 3(\dot{\alpha})^2 - \mathrm{Tr}\,[(\sigma)^2], \tag{A8a}$$

$$R_{11} = \ddot{\alpha} + \dot{\sigma}_{11} + 3(\dot{\alpha})^2 + 3\dot{\alpha}\sigma_{11} + [\sigma,\tau]_{11} + \tfrac{1}{2}e^{-2\alpha}(e^{4\beta}{}_{11} - e^{4\beta}{}_{22} - e^{4\beta}{}_{33} + 2e^{-2\beta}{}_{11}), \tag{A8b}$$

$$R_{0i} = \tfrac{1}{2}e^{-\alpha}[\sigma, e^{2\beta}]_{jk}\epsilon_{ijk}, \tag{A8c}$$

$$R_{12} = \dot{\sigma}_{12} + 3\dot{\alpha}\sigma_{12} + [\sigma,\tau]_{12} + e^{-2\alpha}(e^{4\beta} + e^{-2\beta})_{12}, \tag{A8d}$$

$$R = 6\ddot{\alpha} + 12(\dot{\alpha})^2 + \mathrm{Tr}\,[(\sigma)^2] + e^{-2\alpha}\,\mathrm{Tr}\,(e^{-2\beta} - \tfrac{1}{2}e^{4\beta}), \tag{A8e}$$

with similar expressions for the other R_{ij}. With these quantities at hand, we can form the Einstein equations $R_{\mu\nu} - \frac{1}{2}\eta_{\mu\nu}R = 8\pi T_{\mu\nu}$:

$$8\pi T_{00} = 3(\dot{\alpha})^2 - \tfrac{1}{2}\,\mathrm{Tr}\,[(\sigma)^2] - \tfrac{1}{4}e^{-2\alpha}\,\mathrm{Tr}\,(e^{4\beta} - 2e^{-2\beta}), \tag{A9a}$$

$$8\pi T_{0i} = \tfrac{1}{2}e^{-\alpha}[\sigma, e^{2\beta}]_{jk}\epsilon_{ijk}, \tag{A9b}$$

$$8\pi(T_{11} - \tfrac{1}{3}T_{kk}) = \dot{\sigma}_{11} + 3\dot{\alpha}\sigma_{11} + [\sigma,\tau]_{11} + e^{-2\alpha}[(e^{4\beta} + e^{-2\beta}) - \tfrac{1}{3}\,\mathrm{Tr}\,(e^{4\beta} + e^{-2\beta})], \tag{A9c}$$

$$8\pi T_{12} = \dot{\sigma}_{12} + 3\dot{\alpha}\sigma_{12} + [\sigma,\tau]_{12} + e^{-2\alpha}(e^{4\beta} + e^{-2\beta})_{12}, \tag{A9d}$$

$$\tfrac{8}{3}\pi T_{kk} = -2\ddot{\alpha} - 3(\dot{\alpha})^2 - \tfrac{1}{2}\,\mathrm{Tr}\,[(\sigma)^2] - \tfrac{1}{12}e^{-2\alpha}\,\mathrm{Tr}\,(e^{4\beta} - 2e^{-2\beta}). \tag{A9e}$$

Once we have these equations in this frame, we can define the matrix B by $B = A(t)e^{\beta}$, after Misner,[13] with $A^TA = 1$ and $\dot{A} = -A\tau$. This definition makes $\dot{B}B^{-1}$ symmetric. If we now define $R = e^{\alpha}$ and $S_{ij} = (\dot{B}B^{-1})R^3$ and transform to an orthonormal frame whose basis vectors are $\omega' = A\omega$, the Einstein equations take the form of Eqs. (7a)–(7d).

APPENDIX B

In this appendix we wish to present expressions for $U'^{\mu} = U^{\mu}{}_{;\nu}U^{\nu}$. If we write $\mathbf{U} = U^{\mu}\mathbf{e}_{\mu}$ with the $\mathbf{e}_{\mu}$ the basis vectors dual to the forms (dt, σ_i), then

$$d\mathbf{U} = dU^{\mu}\mathbf{e}_{\mu} + U^{\mu}\omega_{\mu}{}^{\nu}\mathbf{e}_{\nu} = \dot{U}^{\mu}\omega^{0}\mathbf{e}_{\mu} + U^{\mu}\omega_{\mu}{}^{\nu}e_{\nu}.$$

If we allow this vector-valued form to operate on $\mathbf{U}$, we get $d\mathbf{U}(\mathbf{U}) = U^{\mu}{}_{;\nu}U^{\mu}\mathbf{e}_{\mu}$. Inserting $\omega^{\mu}{}_{\nu}$ from Appendix A, we find, in the orthonormal frame of that appendix,

$$d\mathbf{U}(\mathbf{U}) = \gamma\dot{\gamma}\mathbf{e}_0 + \dot{U}_i\gamma\mathbf{e}_i + \gamma(\dot{\alpha}\delta^i_j + \sigma_{ij})U^j\mathbf{e}_i + U_i(\dot{\alpha}\delta^i_j + \sigma_{ij})U^j\mathbf{e}_0 - U_i\gamma\tau_{ij}\mathbf{e}_j + U_kU_m\Gamma_{jkm}\mathbf{e}_j, \tag{B1}$$

which implies that

$$U'^{0} = \dot{\gamma}\gamma + \dot{\alpha}(\gamma^2 - 1) + \sigma_{ij}U_iU_j, \tag{B2a}$$

$$U'^{i} = \gamma\dot{U}_i + \gamma\dot{\alpha}U_i + \gamma(\sigma + \tau)_{ij}U_j + \Gamma_{ijk}U_jU_k. \tag{B2b}$$

Transforming to the frame $\omega' = A\omega$, we find that

$$U'^{0} = \dot{\gamma}\gamma + (\dot{R}/R)(\gamma^2 - 1) + R^{-3}S_{ij}U_iU_j, \tag{B3a}$$

$$U'^{i} = \gamma\dot{U}_i + \gamma(\dot{R}/R)U_i + \gamma R^{-3}S_{ij}U_j - R^{-1}[(B^{\mathrm{T}}B)_{jl}U_kU_j\epsilon_{ikl}]. \tag{B3b}$$

APPENDIX C

In the above work we made use of conservation of energy and momentum in the form $T^{\mu\nu}{}_{;\nu} = 0$. We might hope that there were other conservation laws related to the conservation of angular momentum and circulation (the law of conservation of circulation or Kelvin's theorem is discussed by Landau and Lifshitz).[25]

If we define[27] the differential one-form

$$C = [(\epsilon + p)/n]U_{\mu}\omega^{\mu}$$

and the two-form

$$W_{\mu\nu}\omega^{\mu} \wedge \omega^{\nu} = dC = [(\epsilon + p)/n]\Omega_{\mu\nu}\omega^{\mu} \wedge \omega^{\nu},$$

we have for isentropic flow

$$\pounds_C(W) = 0,$$

which is given in Ref. 27. In certain cases this could lead to a conservation law for W and hence for Ω.

If we make the generalization of $\Gamma = \oint v \cdot dl$ (see Ref. 24) to $\Gamma = \int_{\partial M} C$, where ∂M is the boundary of some three-submanifold in any one t = const surface, we find that in the notation of Lichnerowicz

$$\pounds_C\Gamma = \pounds_C\int_{\partial M} C = \int_{\partial M}\pounds_C C = \int_{\partial M}\{d[\mathbf{i}(C)C] + \mathbf{i}(C)dC\},$$

and, because the second term in the integral is zero, by Stokes' theorem we have

$$\pounds_C\Gamma = \int_{\partial(\partial M)}\mathbf{i}(C)C = 0.$$

In our case neither of these relations leads to simple conservation laws.

[27] A. Lichnerowicz, *Relativistic Hydrodynamics and Magnetohydrodynamics* (W. A. Benjamin, Inc., New York, 1967), Chap. 2.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Concerning the Zeros of Some Functions Related to Bessel Functions*

TIMOTHY H. BOYER†
Harvard University, Cambridge, Massachusetts

(Received 28 November 1967)

The real zeros of the Riccati–Bessel functions $(\frac{1}{2}\pi x)^{\frac{1}{2}}J_\nu(x)$, $(\frac{1}{2}\pi x)^{\frac{1}{2}}Y_\nu(x)$, of their derivatives

$$d[(\tfrac{1}{2}\pi x)^{\frac{1}{2}}J_\nu(x)]/dx, \quad d[(\tfrac{1}{2}\pi x)^{\frac{1}{2}}Y_\nu(x)]/dx,$$

and of their cross products $\frac{1}{2}\pi x[J_\nu(x)Y_\nu(Kx) - Y_\nu(x)J_\nu(Kx)]$,

$$\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right]\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(Kx)\right] - \frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x)\right]\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(Kx)\right]$$

are investigated. Expansions analogous to those provided by McMahon and Olver for the zeros of the Bessel functions are obtained for the zeros of the derivatives of the Riccati–Bessel functions. The analysis of Kalähne for the zeros of the cross product of Bessel functions is considerably expanded and analogous results are obtained for the zeros of the cross product of the derivatives of the Riccati–Bessel functions. Included are derivations of the expansions for large zeros at fixed ν, of asymptotic expansions for large ν at fixed number of the zero, and also asymptotic expansions for the zeros as $K \to 1$ and $K \to \infty$. Figures illustrating the behavior of the zeros are provided for $\nu = l + \frac{1}{2}$, where l is an integer. These zeros correspond to the *TE* and *TM* electromagnetic normal modes inside a conducting spherical shell and in the region between two concentric conducting shells.

INTRODUCTION

The Functions to be Considered

Although the literature concerning the zeros of Bessel functions is considerable (including a chapter in Watson's famous work[1] and extensive new work by Olver[2]) there are still many gaps in the information about the zeros of related functions of interest in physical problems. During recent research regarding the zero-point energy of the quantum electromagnetic field, the author found he required a knowledge of the zeros of the Riccati–Bessel functions $xj_l(x)$ and derivatives $d[xj_l(x)]/dx$, which zeros correspond to the frequencies for transverse electric and magnetic normal modes in a spherical cavity with conducting walls, and also of the zeros of

$$\frac{xj_l(x)}{xy_l(x)} - \frac{xj_l(Kx)}{xy_l(Kx)} \quad \text{and} \quad \frac{\frac{d}{dx}(xj_l(x))}{\frac{d}{dx}(xy_l(x))} - \frac{\frac{d}{dx}(xj_l(Kx))}{\frac{d}{dx}(xy_l(Kx))},$$

corresponding to the frequencies of the modes in the region between two concentric conducting spherical shells. A search of the literature concerning these zeros revealed scant information for the last three functions. This paper is the result of the author's investigations into the properties of the zeros of these functions.

Section 1 deals with the zeros of $(\frac{1}{2}\pi x)^{\frac{1}{2}}J_\nu(x)$, $(\frac{1}{2}\pi x)^{\frac{1}{2}}Y_\nu(x)$, and

$$\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right], \quad \frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x)\right],$$

where we have chosen to emphasize the generality of the analysis by writing the functions in terms of the more familiar cylindrical Bessel functions rather than the spherical Bessel functions. We sketch the results in the published literature regarding the zeros of $J_\nu(x)$, $Y_\nu(x)$, and then derive analogous results for the zeros of the derivatives of the Riccati–Bessel functions, including expansions when the number of the zero becomes large, following the work of McMahon,[3] and asymptotic expansions in the order ν for fixed number of the zero. In Sec. 2 we turn to the zeros of

$$\frac{J_\nu(x)}{Y_\nu(x)} - \frac{J_\nu(Kx)}{Y_\nu(Kx)}$$

and

$$\frac{\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right]}{\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x)\right]} - \frac{\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(Kx)\right]}{\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(Kx)\right]},$$

extending the work of Kalähne[4] in regard to the

* Research supported in part by the Office of Naval Research Nonr 1866(55).

† Present address: Center for Theoretical Physics, Department of Physics and Astronomy, University of Maryland, College Park, Md. 20742.

[1] G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, Cambridge, England, 1952).

[2] F. W. J. Olver (a) Proc. Cambridge Phil. Soc. **46**, 570 (1950); (b) **47**, 699 (1951); (c) **48**, 414 (1952); (d) *Royal Society Mathematical Tables, Vol. 7: Bessel Functions Part III, Zeros and Associated Values*, F. W. J. Olver, Ed. (Cambridge University Press, Cambridge, England, 1960).

[3] J. McMahon, Ann. Math. **9**, 23 (1895).

[4] A. Kalähne, Z. Math. Phys. **54**, 55 (1907).

former function and then developing analogous results for the zeros of the latter. Included are derivations of the expansions for the large zeros at fixed order ν, of asymptotic expansions for large ν at fixed number of zero, and also of asymptotic expansions for the zeros as $K \to 1$ and $K \to \infty$. Figures illustrating the dependence of the zeros on the various parameters are provided for $\nu = l + \frac{1}{2}$, where l is integral.

Notation

The notation[5] of this paper is essentially that of Watson[1] with some additions introduced by Olver.[2] The cylindrical Bessel functions[6] $J_\nu(x)$, $Y_\nu(x)$ are solutions of the Bessel differential equation

$$\frac{d^2W}{dx^2} + \frac{1}{x}\frac{dW}{dx} + \left(1 - \frac{\nu^2}{x^2}\right)W = 0 \tag{1}$$

with

$$J_\nu(x) = \left(\frac{x}{2}\right)^\nu \sum_{r=0}^{\infty} \frac{(-1)^r(\frac{1}{2}x)^{2r}}{r!\,(\nu + r)!} \tag{2}$$

and

$$Y_\nu(x) = \frac{J_\nu(x)\cos\pi\nu - J_{-\nu}(x)}{\sin\pi\nu}, \tag{3}$$

where for integral $\nu = n$, $Y_n(x)$ is defined as the limit of the above expression as $\nu \to n$. A general real cylinder function is a multiple of

$$\mathcal{C}_{\nu,t}(x) = J_\nu(x)\cos\pi t + Y_\nu(x)\sin\pi t, \tag{4}$$

where t is a real parameter independent of ν and x.

The spherical Bessel functions[7] of order l, $j_l(x)$, $y_l(x)$ are related to the cylindrical Bessel functions by

$$j_l(x) = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} J_{l+\frac{1}{2}}(x), \quad y_l(x) = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} Y_{l+\frac{1}{2}}(x) \tag{5}$$

and satisfy the differential equation

$$\frac{d^2w}{dx^2} + \frac{2}{x}\frac{dw}{dx} + \left[1 - \frac{l(l+1)}{x^2}\right]w = 0. \tag{6}$$

The Riccati–Bessel functions, for which no special notation seems to have been introduced, are related to the spherical Bessel functions by $xj_l(x)$, $xy_l(x)$, or to the cylindrical Bessel functions by $(\frac{1}{2}\pi x)^{\frac{1}{2}}J_{l+\frac{1}{2}}(x)$, $(\frac{1}{2}\pi x)^{\frac{1}{2}}Y_{l+\frac{1}{2}}(x)$. These satisfy the differential equation

$$\frac{d^2\omega}{dx^2} + \left[1 - \frac{l(l+1)}{x^2}\right]\omega = 0. \tag{7}$$

The zeros of the cross products considered in Sec. 2,

$$\frac{J_\nu(x)}{Y_\nu(x)} - \frac{J_\nu(Kx)}{Y_\nu(Kx)}, \tag{8}$$

$$\frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x)\right]} - \frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(Kx)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(Kx)\right]} \tag{9}$$

are the same as those of

$$J_\nu(x)Y_\nu(Kx) - Y_\nu(x)J_\nu(Kx), \tag{10}$$

$$\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right]\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(Kx)\right] - \frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x)\right]\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(Kx)\right], \tag{11}$$

and, using Eq. (3), as those of

$$J_\nu(x)J_{-\nu}(Kx) - J_{-\nu}(x)J_\nu(Kx), \tag{12}$$

$$\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right]\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_{-\nu}(Kx)\right] - \frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_{-\nu}(x)\right]\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(Kx)\right]. \tag{13}$$

The forms (8), (10), and (12) all appear in the literature.

The notation for the zeros again follows that of the work in Watson, Olver, and, in part, that of Kalähne. For nonnegative ν, the real zeros of $J_\nu(x)$, $Y_\nu(x)$, $J'_\nu(x)$, $Y'_\nu(x)$ are denoted, respectively, by $j_{\nu,s}$, $y_{\nu,s}$, $j'_{\nu,s}$, $y'_{\nu,s}$, where s is an integer index which for fixed ν labels the positive zeros in order of increasing magnitude, except (following a modification by Olver) $j'_{0,1} = 0$. Since there seems to be no standard notation for the zeros of the Riccati–Bessel functions, we denote the positive zeros of

$$\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x), \quad \left(\frac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x),$$

$$\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right], \quad \frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x)\right]$$

by, respectively, $\bar{j}_{\nu,s}$, $\bar{y}_{\nu,s}$, $\bar{j}'_{\nu,s}$, $\bar{y}'_{\nu,s}$. When the functions $xj_l(x)$, $xy_l(x)$ are involved, we use the above notations with $\nu = l + \frac{1}{2}$.

Olver has introduced the notations[8] $\rho_\nu(t)$ and $\sigma_\nu(t)$ for the zeros of $\mathcal{C}_{\nu,t}(x)$ and $\mathcal{C}'_{\nu,t}(x)$ as continuous functions of t. If we require $\rho_\nu(0) = 0$ and $\sigma_\nu(0) = j'_{\nu,1}$, then

$$j_{\nu,s} = \rho_\nu(s), \qquad y_{\nu,s} = \rho(s - \tfrac{1}{2}),$$
$$j'_{\nu,s} = \sigma_\nu(s - 1), \quad y'_{\nu,s} = \sigma_\nu(s - \tfrac{1}{2}), \tag{14}$$

[5] There is a confusing variety of notations, especially in the older literature, with symbols sometimes being interchanged from what is more common today. See *The British Association for the Advancement of Science Mathematical Tables, Vol. 10, Bessel Functions Part II* (Cambridge University Press, Cambridge, England, 1952). This book devotes p. xxx to summarizing some of the notations.

[6] P. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Co., Inc., New York, 1953). Substitute $N_\nu(x)$ for $Y_\nu(x)$.

[7] The spherical Neumann function $y_l(x)$ is something denoted by $n_l(x)$; e.g., in Ref. 6.

[8] Actually, $\rho_\nu(-t)$ and $\sigma_\nu(-t)$ are what Olver has called $\rho(\nu, t)$ and $\sigma(\nu, t)$. Thus when Olver speaks of negative values of t, we will speak of positive values.

for positive integral s. The notations for the Riccati–Bessel functions follow in the same manner, as above, so that $\bar{\rho}_\nu(t)$ and $\bar{\sigma}_\nu(t)$ denote zeros of

$$\left(\frac{\pi x}{2}\right)^{\frac{1}{2}} \mathcal{C}_{\nu,t}(x) \quad \text{and} \quad \frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}} \mathcal{C}_{\nu,t}(x)\right],$$

respectively. Again we normalize $\bar{\rho}_\nu(0) = 0$ and $\bar{\sigma}_\nu(0) = \bar{j}'_{\nu,1}$, and for $\nu \geq \frac{1}{2}$ find

$$\begin{aligned} \bar{j}_{\nu,s} &= \bar{\rho}_\nu(s), & \bar{y}_{\nu,s} &= \bar{\rho}_\nu(s - \tfrac{1}{2}), \\ \bar{j}'_{\nu,s} &= \bar{\sigma}_\nu(s - 1), & \bar{y}'_{\nu,s} &= \bar{\sigma}_\nu(s - \tfrac{1}{2}). \end{aligned} \tag{15}$$

When $0 \leq \nu < \frac{1}{2}$, $d[(\frac{1}{2}\pi x)^{\frac{1}{2}} Y_\nu(x)]/dx$ has one additional positive zero below $\bar{\sigma}_\nu(\frac{1}{2})$ considered as a continuous function of ν.

The positive zeros of

$$\frac{J_\nu(x)}{Y_\nu(x)} - \frac{J_\nu(Kx)}{Y_\nu(Kx)}$$

and of

$$\frac{J'_\nu(x)}{Y'_\nu(x)} - \frac{J'_\nu(Kx)}{Y'_\nu(Kx)}, \quad K > 1,$$

are here indicated by $x_{\nu,K,s}$ and $x'_{\nu,K,s}$ when s is an integer index labeling the zeros in order of increasing magnitude. The positive zeros of

$$\frac{(\frac{1}{2}\pi x)^{\frac{1}{2}} J_\nu(x)}{(\frac{1}{2}\pi x)^{\frac{1}{2}} Y_\nu(x)} - \frac{(\frac{1}{2}\pi x)^{\frac{1}{2}} J_\nu(Kx)}{(\frac{1}{2}\pi x)^{\frac{1}{2}} Y_\nu(Kx)}$$

and

$$\frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}} J_\nu(x)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}} Y_\nu(x)\right]} - \frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}} J_\nu(Kx)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}} Y_\nu(Kx)\right]}$$

are indicated in a notation analogous to that above by $\bar{x}_{\nu,K,s}$, $\bar{x}'_{\nu,K,s}$. Although it is again possible to consider the comparable expressions for the general cylinder function $\mathcal{C}_{\nu,t}(x)$ instead of $J_\nu(x)$, for example,

$$\frac{\mathcal{C}_{\nu,t}(x)}{\mathcal{C}_{\nu,t+\frac{1}{2}}(x)} - \frac{\mathcal{C}_{\nu,t}(Kx)}{\mathcal{C}_{\nu,t+\frac{1}{2}}(Kx)}, \tag{16}$$

the zeros are the $x_{\nu,K,s}$ above, and are entirely independent of t. This is easily seen by noting

$$\begin{aligned} \mathcal{C}_{\nu,t}(x)\mathcal{C}_{\nu,t+\frac{1}{2}}(Kx) - \mathcal{C}_{\nu,t+\frac{1}{2}}(x)\mathcal{C}_{\nu,t}(Kx) \\ = J_\nu(x)Y_\nu(Kx) - Y_\nu(x)J_\nu(Kx). \end{aligned} \tag{17}$$

Hence, no further notation for the zeros needs to be introduced.

1. ZEROS OF THE RICCATI–BESSEL FUNCTIONS AND DERIVATIVES

Zeros of the Bessel Functions

The behavior of the Riccati–Bessel functions is illustrated in Fig. 1 for $l = 0, 2, 5$. For $l = 0$, $xj_0(x) = \sin x$ and $xy_0(x) = -\cos x$. If $l > 0$, the function

$$xj_l(x) \to \frac{x^{l+1}}{1 \cdot 3 \cdot 5 \cdots (2l+1)}$$

and

$$xy_l(x) \to \frac{-1 \cdot 3 \cdot 5 \cdots (2l-1)}{x^l}$$

for $x \to 0$. For $x \to \infty$, the functions oscillate as $xj_l(x) \sim \sin(x - \frac{1}{2}\pi l)$, $xy_l(x) \sim -\cos(x - \frac{1}{2}\pi l)$. This summary of some of the properties of these functions is already sufficient to suggest a great deal about the qualitative nature of the zeros. However, inasmuch as

$$xj_l(x) = (\tfrac{1}{2}\pi x)^{\frac{1}{2}} J_{l+\frac{1}{2}}(x), \quad xy_l(x) = (\tfrac{1}{2}\pi x)^{\frac{1}{2}} Y_{l+\frac{1}{2}}(x), \tag{18}$$

the zeros of the Riccati–Bessel functions are the same as those of the related cylindrical Bessel functions $J_\nu(x)$, $Y_\nu(x)$. Hence it is sufficient to recall[9] the information about the zeros of the cylinder functions.

For real order ν, $J_\nu(x)$, $J'_\nu(x)$ have an infinite number of zeros all of which are real; $Y_\nu(x)$, $Y'_\nu(x)$ have infinite numbers of both real and complex zeros. All the zeros are simple except for zeros $x = 0$. The zeros are interlaced according to the inequalities

$$j_{\nu,1} < j_{\nu+1,1} < j_{\nu,2} < j_{\nu+1,2} < j_{\nu,3} < \cdots, \tag{19}$$

$$y_{\nu,1} < y_{\nu+1,1} < y_{\nu,2} < y_{\nu+1,2} < y_{\nu,3} < \cdots, \tag{20}$$

$$\begin{aligned} \nu \leq j'_{\nu,1} < y_{\nu,1} < y'_{\nu,1} < j_{\nu,1} < j'_{\nu,2} \\ < y_{\nu,2} < y'_{\nu,2} < j_{\nu,2} < j'_{\nu,3} < \cdots. \end{aligned} \tag{21}$$

Figure 2 shows the low zeros $j_{l+\frac{1}{2},s}$ for $l = 0(1)20$,

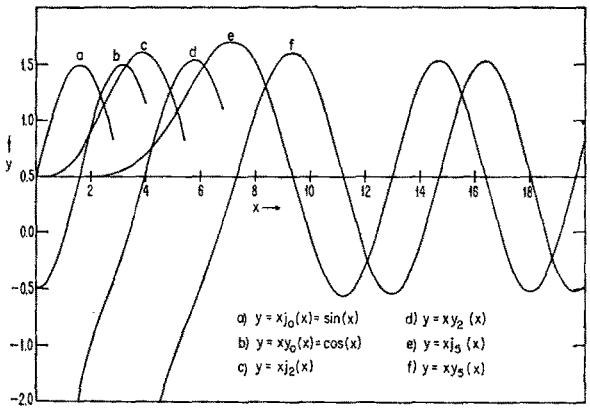


FIG. 1. Graphs of the Riccati–Bessel functions $xj_l(x)$, $xy_l(x)$, $l = 0, 2, 5$. The curves show the behavior of $xj_l(x)$, $xy_l(x)$ for $l = 0, 2, 5$ for small values of x. The curves for $l = 5$ are shown over an extended range so as to indicate their approach to functions with sine and cosine oscillations.

[9] Excellent short reviews of these zeros are presented in the *Handbook of Mathematical Functions* [M. Abramowitz and J. Stegun, Eds. (Dover Publications, New York, 1965), pp. 370–374, 440–442] and in the introduction to Ref. 2(d).

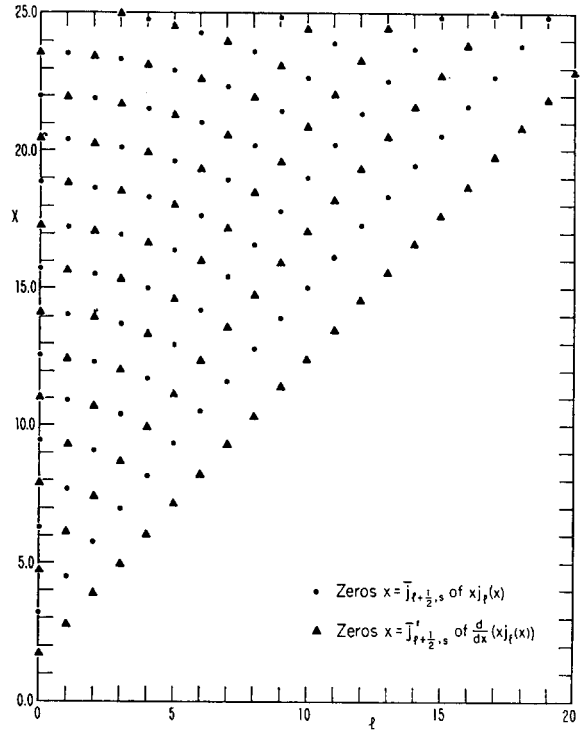


FIG. 2. Zeros of $xj_t(x)$ and $d(xj_t(x))/dx$.

and allows graphical illustration of part of the interlacing pattern. For the general real-cylinder function $\mathcal{C}_{\nu,t}(x)$, the positive zeros are interlaced with the zeros of $\mathcal{C}_{\nu+1,t}(x)$. Also, the positive zeros of any two distinct cylinder functions of the same order ν are interlaced.

McMahon Expansions of the Zeros for Large Numbers

When the argument x becomes large compared to ν, the functions $J_\nu(x)$, $Y_\nu(x)$, $\mathcal{C}_{\nu,t}(x)$ approach asymptotically

$$\begin{aligned} J_\nu(x) &\sim (2/\pi x)^{\frac{1}{2}} \cos [x - \tfrac{1}{2}\pi(\nu + \tfrac{1}{2})], \\ Y_\nu(x) &\sim (2/\pi x)^{\frac{1}{2}} \sin [x - \tfrac{1}{2}\pi(\nu + \tfrac{1}{2})], \\ \mathcal{C}_{\nu,t}(x) &\sim (2/\pi x)^{\frac{1}{2}} \cos [x - \tfrac{1}{2}\pi(\nu + \tfrac{1}{2}) - \pi t] \end{aligned} \tag{22}$$

and, hence, the zeros become those of the corresponding trigonometric functions. McMahon[3] has provided the expansions[10] for the zeros when the number s exceeds the order ν, $s \gg \nu$:

$$\begin{aligned} &j_{\nu,s},\ y_{\nu,s},\ \rho_\nu(t) \\ &\sim \beta - \frac{(\mu-1)}{8\beta} - \frac{(\mu-1)(7\mu-31)}{3!\,8^2\beta^3} \\ &\quad - \frac{4(\mu-1)(83\mu^2 - 982\mu + 3779)}{5!\,8^3\beta^5} + \cdots, \end{aligned} \tag{23}$$

where $\mu = 4\nu^2$, $\beta = \pi(s + \frac{1}{2}\nu - \frac{1}{4})$ for $j_{\nu,s}$; $\beta = \pi(s + \frac{1}{2}\nu - \frac{3}{4})$ for $y_{\nu,s}$; and $\beta = \pi(\frac{1}{2}\nu - \frac{1}{4} + t)$ for $\rho_\nu(t)$. For the spherical Bessel functions, we merely set $l = \nu - \frac{1}{2}$. In the particular case $l = 0$, all the higher coefficients vanish and $j_{\frac{1}{2},s} = \pi s$, $y_{\frac{1}{2},s} = \pi(s - \frac{1}{2})$.

Olver Asymptotic Expansions for Large ν

Asymptotic expansions for the zeros $j_{\nu,s}$, $y_{\nu,s}$ for fixed s and large ν have been developed systematically by Olver.[2] The zeros of the general cylinder function $\mathcal{C}_{\nu,t}(x)$ can be expanded in decreasing powers of $\nu^{\frac{2}{3}}$:

$$\rho_\nu(t) \sim \nu + \alpha_1(t)\nu^{\frac{1}{3}} + \alpha_2(t)\nu^{-\frac{1}{3}} + \alpha_3(t)\nu^{-1} + \cdots. \tag{24}$$

The first three zeros of $J_\nu(x)$, $Y_\nu(x)$, and the values of the derivative of the associated function are given by Olver[11] as follows:

$$\begin{aligned} j_{\nu,1} &\sim \nu + 1.8557571\nu^{\frac{1}{3}} + 1.033150\nu^{-\frac{1}{3}} - 0.00397\nu^{-1} - 0.0908\nu^{-\frac{5}{3}} + \cdots, \\ j_{\nu,2} &\sim \nu + 3.2446076\nu^{\frac{1}{3}} + 3.158244\nu^{-\frac{1}{3}} - 0.08331\nu^{-1} - 0.8437\nu^{-\frac{5}{3}} + \cdots, \\ j_{\nu,3} &\sim \nu + 4.3816712\nu^{\frac{1}{3}} + 5.759713\nu^{-\frac{1}{3}} - 0.22607\nu^{-1} - 2.8039\nu^{-\frac{5}{3}} + \cdots, \end{aligned} \tag{25}$$

$$\begin{aligned} J'_\nu(j_{\nu,1}) &\sim -1.1131028\nu^{-\frac{2}{3}}/(1 + 1.484606\nu^{-\frac{2}{3}} + 0.43294\nu^{-\frac{4}{3}} - 0.1943\nu^{-2} + \cdots), \\ J'_\nu(j_{\nu,2}) &\sim +1.2748598\nu^{-\frac{2}{3}}/(1 + 2.595686\nu^{-\frac{2}{3}} + 1.32345\nu^{-\frac{4}{3}} - 1.0687\nu^{-2} + \cdots), \\ J'_\nu(j_{\nu,3}) &\sim -1.3734258\nu^{-\frac{2}{3}}/(1 + 3.505337\nu^{-\frac{2}{3}} + 2.41359\nu^{-\frac{4}{3}} - 2.6423\nu^{-2} + \cdots), \end{aligned} \tag{26}$$

$$\begin{aligned} y_{\nu,1} &\sim \nu + 0.9315768\nu^{\frac{1}{3}} + 0.260351\nu^{-\frac{1}{3}} + 0.01198\nu^{-1} - 0.0060\nu^{-\frac{5}{3}} - \cdots, \\ y_{\nu,2} &\sim \nu + 2.5962685\nu^{\frac{1}{3}} + 2.022183\nu^{-\frac{1}{3}} - 0.03572\nu^{-1} - 0.3463\nu^{-\frac{5}{3}} + \cdots, \\ y_{\nu,3} &\sim \nu + 3.8341592\nu^{\frac{1}{3}} + 4.410233\nu^{-\frac{1}{3}} - 0.14676\nu^{-1} - 1.6444\nu^{-\frac{5}{3}} + \cdots, \end{aligned} \tag{27}$$

$$\begin{aligned} Y'_\nu(y_{\nu,1}) &\sim +0.9555486\nu^{-\frac{2}{3}}/(1 + 0.745261\nu^{-\frac{2}{3}} + 0.10910\nu^{-\frac{4}{3}} - 0.0185\nu^{-2} - \cdots), \\ Y'_\nu(y_{\nu,2}) &\sim -1.2069171\nu^{-\frac{2}{3}}/(1 + 2.077015\nu^{-\frac{2}{3}} + 0.84739\nu^{-\frac{4}{3}} - 0.5441\nu^{-2} + \cdots), \\ Y'_\nu(y_{\nu,3}) &\sim +1.3286404\nu^{-\frac{2}{3}}/(1 + 3.067327\nu^{-\frac{2}{3}} + 1.84810\nu^{-\frac{4}{3}} - 1.7681\nu^{-2} + \cdots). \end{aligned} \tag{28}$$

[10] Four additional terms in the expansion are given in Ref. 2(d).
[11] Olver [Ref. 2(d), p. xviii] provides additional terms. Expansions for $s = 4$ and 5 are provided in Ref. 2(b).

The values of the derivatives of the spherical Bessel functions or Riccati–Bessel functions at the zeros of these functions may be found directly from Eqs. (5) and (18) relating these functions to the cylindrical Bessel functions, and from Eqs. (26) and (28) giving the values of the derivatives of the cylindrical Bessel functions at these same zeros. Thus, for example,

$$[d(xj_l(x))/dx]_{x=j_{l+\frac{1}{2},s}} = (\tfrac{1}{2}\pi j_{l+\frac{1}{2},s})^{\frac{1}{2}} J'_{l+\frac{1}{2}}(j_{l+\frac{1}{2},s}). \quad (29)$$

A visualization of the behavior of the zeros $j_{\nu,s}$ for changing ν and s may be obtained from Fig. 2 where $j_{l+\frac{1}{2},s}$ is plotted for $l = 0(1)20$, $j_{l+\frac{1}{2},s} < 25.0$. The zeros for small s are given by $\sim\nu + \alpha\nu^{\frac{1}{3}}$, but the gap between low zeros for ν fixed increases with increasing ν. For ν fixed and the number of the zero increasing, the spacing between the zeros decreases steadily toward π. See also Figs. 5, 6, and 7, where the Bessel function zeros appear as limiting cases.

Zeros of the Derivatives of the Riccati–Bessel Functions

There is no immediate relation between the zeros of $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}J_\nu(x)]/dx$, $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}Y_\nu(x)]/dx$ and the zeros of $J'_\nu(x)$, $Y'_\nu(x)$. Thus, we can not in this case shift the problem over to a review of the zeros of well-known functions. However, we still expect the behavior of the zeros of the two sets of functions mentioned above to be quite analogous in all qualitative aspects. The positive zeros $j'_{\nu,s}$, $\bar{y}'_{\nu,s}$ of the Riccati–Bessel functions are again simple and interlaced for adjacent orders and for distinct functions. Figure 2 shows the low zeros $j'_{l+\frac{1}{2},s}$ $l = 0(1)20$ plotted on the same graph as the zeros $j_{l+\frac{1}{2},s} = \bar{j}_{l+\frac{1}{2},s}$. It is clear that the zeros join neatly into a uniform pattern.

Expansions for Large Number of the Zeros

The expansions for large zeros for fixed order ν may be obtained in exactly the style of McMahon. The later and more sophisticated derivation favored by Watson[12] does not seem to be available here since the functional relations analogous to those on which Watson depends do not seem to have been developed yet for $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}J_\nu(x)]/dx$ and $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}Y_\nu(x)]/dx$. The expansions for the cylindrical Bessel functions in descending powers of x give

$$(\tfrac{1}{2}\pi x)^{\frac{1}{2}}J_\nu(x) = \cos[x - \tfrac{1}{2}\pi(\nu + \tfrac{1}{2})]\varphi_\nu(x) + \sin[x - \tfrac{1}{2}\pi(\nu + \tfrac{1}{2})]\psi_\nu(x), \quad (30)$$

$$(\tfrac{1}{2}\pi x)^{\frac{1}{2}}Y_\nu(x) = -\cos[x - \tfrac{1}{2}\pi(\nu + \tfrac{1}{2})]\psi_\nu(x) + \sin[x - \tfrac{1}{2}\pi(\nu + \tfrac{1}{2})]\varphi_\nu(x), \quad (31)$$

where

$$\varphi_\nu(x) = 1 - \frac{(\mu - 1^2)(\mu - 3^2)}{2!\,(8x)^2} + \frac{(\mu - 1^2)(\mu - 3^2)(\mu - 5^2)(\mu - 7^2)}{4!\,(8x)^4} - \cdots, \quad (32)$$

$$\psi_\nu(x) = -\frac{\mu - 1}{8x} + \frac{(\mu - 1^2)(\mu - 3^2)(\mu - 5^2)}{3!\,(8x)^3} - \cdots. \quad (33)$$

Then

$$\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right] = -\sin\left[x - \frac{\pi}{2}(\nu + \tfrac{1}{2})\right](\varphi_\nu(x) - \psi'_\nu(x)) + \cos\left[x - \frac{\pi}{2}(\nu + \tfrac{1}{2})\right](\psi_\nu(x) + \varphi'_\nu(x)), \quad (34)$$

$$\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x)\right] = \sin\left[x - \frac{\pi}{2}(\nu + \tfrac{1}{2})\right](\psi_\nu(x) + \varphi'_\nu(x)) + \cos\left[x - \frac{\pi}{2}(\nu + \tfrac{1}{2})\right](\varphi_\nu(x) - \psi'_\nu(x)). \quad (35)$$

If we introduce the general cylinder function $C_{\nu,t}(x)$ as in Eq. (4), then, from Eqs. (30) and (31), the zeros of $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}C_{\nu,t}(x)]/dx$ are given by

$$\tan\left[x - \frac{\pi}{2}(\nu + \tfrac{1}{2}) - \pi t\right] = \frac{\psi_\nu(x) + \varphi'_\nu(x)}{\varphi_\nu(x) - \psi'_\nu(x)}. \quad (36)$$

Following McMahon, we expand

$$\arctan\left(\frac{\psi_\nu(x) + \varphi'_\nu(x)}{\varphi_\nu(x) - \psi'_\nu(x)}\right)$$

in descending powers of x. Then the sth zero (here restricting t to lie in $[0, \frac{1}{2}]$) satisfies

$$\begin{aligned} x - \frac{\pi}{2}(\nu + \tfrac{1}{2}) - \pi t &= \pi(s - 1) + \left(\frac{\psi_\nu(x) + \varphi'_\nu(x)}{\varphi_\nu(x) - \psi'_\nu(x)}\right) - \frac{1}{3}\left(\frac{\psi_\nu(x) + \varphi'_\nu(x)}{\varphi_\nu(x) - \psi'_\nu(x)}\right)^3 + \frac{1}{5}\left(\frac{\psi_\nu(x) + \varphi'_\nu(x)}{\varphi_\nu(x) - \psi'_\nu(x)}\right)^5 - \cdots \\ &= \pi(s - 1) - \frac{\mu - 1}{8x} - \frac{(\mu - 1)(8\mu + 184)}{3!\,(8x)^3} - \frac{(\mu - 1)(768\mu^2 + 96768\mu - 834816)}{5!\,(8x)^5} - \cdots. \end{aligned} \quad (37)$$

[12] Reference 1, p. 505.

Using Lagrange's theorem,[13]

$$x \sim \beta - \frac{(\mu-1)}{8\beta} - \frac{(\mu-1)(7\mu+17)}{3!\,8^2\beta^3} - \frac{4(\mu-1)(83\mu^2+698\mu-3661)}{5!\,8^3\beta^5} - \cdots, \quad (38)$$

where $\beta = \pi(s + \frac{1}{2}\nu - \frac{3}{4} + t)$, $0 \le t \le \frac{1}{2}$. Separating out the various Bessel and Neumann forms, we get

$$\begin{aligned}
&\beta = \pi(s + \tfrac{1}{2}\nu - \tfrac{3}{4}) \quad \text{for} \quad j'_{\nu,s};\\
&\beta = \pi(s + \tfrac{1}{2}\nu - \tfrac{1}{4}) \quad \text{for} \quad \bar{y}'_{\nu,s}, \quad \nu \ge \tfrac{1}{2};\\
&\beta = \pi(s + \tfrac{1}{2}\nu - \tfrac{5}{4}) \quad \text{for} \quad \bar{y}'_{\nu,s}, \quad 0 \le \nu < \tfrac{1}{2};\\
&\beta = \pi(t + \tfrac{1}{2}\nu - \tfrac{1}{4}) \quad \text{for} \quad \bar{\sigma}'_{\nu}(t), \quad 0 \le t.
\end{aligned}$$

Asymptotic Expansions for Large Order ν

If we write out

$$\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}} J_\nu(x)\right] = \left(\frac{\pi x}{2}\right)^{\frac{1}{2}}\left(J'_\nu(x) + \frac{1}{2x} J_\nu(x)\right) \quad (39)$$

and recall[14] that $|J_\nu(x)|$ is bounded by $O(\nu^{-\frac{1}{3}})$ while $|J'_\nu(x)|$ is $O(\nu^{-\frac{2}{3}})$, it is clear that for large x the zeros of $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}J_\nu(x)]/dx$ approach those of $J'_\nu(x)$. Thus in the expansion derived above in Eq. (38) for the sth zero $s \gg \nu$, the first two terms in the expansion are identical with those found by McMahon[3] for the zeros of $J'_\nu(x)$. Also, since the first zero $j'_{\nu,1}$ of $J'_\nu(x)$ is larger than ν and both $J'_\nu(x)$ and $(2x)^{-1}J_\nu(x)$ are positive for $0 < x < j'_{\nu,1}$, and further since

$$|(2x)^{-1}J_\nu(x)| < O(\nu^{-\frac{4}{3}}) \quad \text{for} \quad x > \nu,$$

it follows that *all* the zeros of $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}J_\nu(x)]/dx$ approach those of $J'_\nu(x)$ for large ν. Thus we must have $J'_{\nu,s} \sim \nu + \alpha_{1,s}\nu^{\frac{1}{3}} + \epsilon$, where $\alpha_{1,s}$ coincides with the coefficient for the expansion of the zeros $j'_{\nu,s}$ of $J'_\nu(x)$ and $\epsilon \to 0$ as $\nu \to \infty$. An analogous argument can be made for $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}Y_\nu(x)]/dx$ for $\nu > \frac{1}{2}$.

In order to obtain the asymptotic expansions for the zeros as the order $\nu \to \infty$, we take advantage of Olver's expansions[15] for the cylindrical Bessel functions in the region $x = \nu + \tau\nu^{\frac{1}{3}}$:

$$J_\nu^{(m)}(\nu + \tau\nu^{\frac{1}{3}}) \sim \frac{2^{\frac{1}{3}}}{\nu^{\frac{1}{3}(m+1)}}\,\mathrm{Ai}\,(-2^{\frac{1}{3}}\tau) \times \sum_{s=0}^{\infty}\frac{A_s^m(\tau)}{\nu^{\frac{2}{3}s}} + \frac{2^{\frac{2}{3}}}{\nu^{\frac{1}{3}(m+1)}}\,\mathrm{Ai}'\,(-2^{\frac{1}{3}}\tau)\sum_{s=0}^{\infty}\frac{B_s^m(\tau)}{\nu^{\frac{2}{3}s}}, \quad (40)$$

$$Y_\nu^{(m)}(\nu + \tau\nu^{\frac{1}{3}}) \sim -\frac{2^{\frac{1}{3}}}{\nu^{\frac{1}{3}(m+1)}}\,\mathrm{Bi}\,(-2^{\frac{1}{3}}\tau) \times \sum_{s=0}^{\infty}\frac{A_s^m(\tau)}{\nu^{\frac{2}{3}s}} - \frac{2^{\frac{2}{3}}}{\nu^{\frac{1}{3}(m+1)}}\,\mathrm{Bi}'\,(-2^{\frac{1}{3}}\tau)\sum_{s=0}^{\infty}\frac{B_s^m(\tau)}{\nu^{\frac{2}{3}s}}. \quad (41)$$

The superscript m indicates the derivative of the Bessel functions, and $J_\nu^{(0)} \equiv J_\nu$, $Y_\nu^{(0)} \equiv Y_\nu$. The functions Ai and Bi are the Airey integral functions. The coefficients $A_s^m(\tau)$, $B_s^m(\tau)$ are polynomials in τ determined in the derivation of the expansions. The first few coefficients $A_s^0(\tau)$, $B_s^0(\tau)$ are

$$\begin{aligned}
&A_0^0 = 1, \quad A_1^0 = -\tfrac{1}{5}\tau,\\
&A_2^0 = -\tfrac{9}{100}\tau^5 + \tfrac{3}{35}\tau^2,\\
&A_3^0 = \tfrac{957}{7000}\tau^6 - \tfrac{173}{3150}\tau^3 - \tfrac{1}{225},\\
&B_0^0 = 0, \quad B_1^0 = \tfrac{3}{10}\tau^2,\\
&B_2^0 = -\tfrac{17}{70}\tau^3 + \tfrac{1}{70},\\
&B_3^0 = -\tfrac{9}{1000}\tau^7 + \tfrac{611}{3150}\tau^4 - \tfrac{37}{3150}\tau,
\end{aligned} \quad (42)$$

and the terms $A_s^m(\tau)$, $B_s^m(\tau)$ may be found from the recurrence relations

$$\begin{aligned}
A_s^{m+1}(\tau) &= \frac{d}{d\tau}A_s^m(\tau) + 2\tau B_s^m(\tau),\\
B_s^{m+1}(\tau) &= -A_s^m(\tau) + \frac{d}{d\tau}B_s^m(\tau).
\end{aligned} \quad (43)$$

Here again, it is quite as easy to handle the general Riccati-Bessel function $(\frac{1}{2}\pi x)^{\frac{1}{2}}\mathcal{C}_{\nu,t}(x)$ as it is to handle the Bessel and Neumann forms individually. We expand $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}\mathcal{C}_{\nu,t}(x)]/dx$ in a Taylor series about $x = \nu + \alpha_1\nu^{\frac{1}{3}}$, and require that it vanish at $x = \nu + \alpha_1\nu^{\frac{1}{3}} + \epsilon$ corresponding to the zero $\bar{\sigma}'_\nu(t)$. Comparing coefficients of powers of ν, we determine the expansion $\epsilon = \alpha_2\nu^{-\frac{1}{3}} + \alpha_3\nu^{-1} + \alpha_4\nu^{-\frac{5}{3}} + \cdots$. Thus

$$\begin{aligned}
0 &= \left\{\frac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}\mathcal{C}_{\nu,t}(x)\right]\right\}_{x=\nu+\alpha_1\nu^{\frac{1}{3}}+\epsilon}\\
&= \sum_{m=0}^{\infty}\frac{\epsilon^m}{m!}\sum_{r=0}^{r=m+1}\frac{(m+1)!}{r!\,(m+1-r)!}(\tfrac{1}{2})(-\tfrac{1}{2})\cdots(\tfrac{1}{2}-r+1)\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}\frac{1}{x^r}\,\mathcal{C}_{\nu,t}^{(m+1-r)}(x)\right]_{x=\nu+\alpha_1\nu^{\frac{1}{3}}}\\
&\sim \sum_{m=0}^{\infty}\frac{\epsilon^m}{m!}\sum_{r=0}^{r=m+1}\frac{(m+1)!}{r!\,(m+1-r)!}(\tfrac{1}{2})(-\tfrac{1}{2})\cdots(\tfrac{1}{2}-r+1)\left[\frac{\pi(\nu+\alpha_1\nu^{\frac{1}{3}})}{2}\right]^{\frac{1}{2}}\frac{1}{(\nu+\alpha_1\nu^{\frac{1}{3}})^r}\\
&\quad\times\left(\frac{2^{\frac{1}{3}}}{\nu^{\frac{1}{3}(m+2-r)}}\left[(\cos\pi t)\,\mathrm{Ai}\,(-2^{\frac{1}{3}}\alpha_1) - (\sin\pi t)\,\mathrm{Bi}\,(-2^{\frac{1}{3}}\alpha_1)\right]\sum_{s=0}^{\infty}\frac{A_s^{m+1-r}(\alpha_1)}{\nu^{\frac{2}{3}s}}\right.\\
&\quad\left.+\frac{2^{\frac{2}{3}}}{\nu^{\frac{1}{3}(m+2-r)}}\left[(\cos\pi t)\,\mathrm{Ai}'\,(-2^{\frac{1}{3}}\alpha_1) - (\sin\pi t)\,\mathrm{Bi}'\,(-2^{\frac{1}{3}}\alpha_1)\right]\sum_{s=0}^{\infty}\frac{B_s^{m+1-r}(\alpha_1)}{\nu^{\frac{2}{3}s}}\right).
\end{aligned} \quad (44)$$

[13] See, for example, E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, Cambridge, England, 1962), pp. 132–133.

[14] We have $J_\nu(j'_{\nu,s}) \sim \nu^{-\frac{1}{3}}$, $J'_\nu(j_{\nu,s}) \sim \nu^{-\frac{2}{3}}$ for large ν. See the expansions, Eqs. (40) and (41) below.

[15] See Ref. 2(c).

Now the coefficient α_1 is determined by the condition

$$(\cos \pi t)\,\mathrm{Ai}'(-2^{\frac{1}{3}}\alpha_1) - (\sin \pi t)\,\mathrm{Bi}'(-2^{\frac{1}{3}}\alpha_1) = 0, \tag{45}$$

which we see from the asymptotic expansions (40) and (41) is the same condition that

$$\mathcal{C}'_{\nu,t}(\nu + \alpha_1\nu^{\frac{1}{3}}) = 0 + O(\nu^{-\frac{4}{3}}). \tag{46}$$

Removing the common factors from (44), we arrive at the equation

$$0 \sim \sum_{m=0}^{\infty} \frac{\epsilon^m}{m!} \sum_{r=0}^{r=m+1} \frac{(m+1)!}{r!\,(m+1-r)!} (\tfrac{1}{2})(-\tfrac{1}{2})\cdots(\tfrac{1}{2}-r+1) \frac{1}{(\nu+\alpha_1\nu^{\frac{1}{3}})^r} \frac{1}{\nu^{\frac{1}{3}(m+2-r)}} \sum_{s=0}^{\infty} \frac{A_s^{m+1-r}(\alpha_1)}{\nu^{\frac{2}{3}s}}. \tag{47}$$

From this expansion, with $\epsilon \sim \alpha_2\nu^{-\frac{1}{3}} + \alpha_3\nu^{-1} + \alpha_4\nu^{-\frac{5}{3}} + \cdots$, we find

$$\begin{aligned} \alpha_2 &= \tfrac{3}{20}\alpha_1^{-1} + \tfrac{3}{10}\alpha_1^2, \quad \alpha_3 = -\tfrac{9}{800}\alpha_1^{-3} + \tfrac{1}{100} - \tfrac{1}{350}\alpha_1^3, \\ \alpha_4 &= \tfrac{27}{160000}\alpha_1^{-5} - \tfrac{9}{4000}\alpha_1^{-2} - \tfrac{1457}{630000}\alpha_1 - \tfrac{479}{630000}\alpha_1^4. \end{aligned} \tag{48}$$

The zeros[16] for the Bessel function form of $\mathcal{C}'_{\nu,t}(x)$ require $0 = \mathrm{Ai}(-2^{\frac{1}{3}}\alpha_1)$ and for the Neumann form $0 = \mathrm{Bi}(-2^{\frac{1}{3}}\alpha_1)$. The asymptotic expansions for the first five zeros $j'_{\nu,s}$ of $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}J_\nu(x)]/dx$ are

$$\begin{aligned} j'_{\nu,1} &\sim \nu + 0.8086165\nu^{\frac{1}{3}} + 0.381660\nu^{-\frac{1}{3}} - 0.01279\nu^{-1} - 0.0205\nu^{-\frac{5}{3}} + \cdots, \\ j'_{\nu,2} &\sim \nu + 2.5780961\nu^{\frac{1}{3}} + 2.052156\nu^{-\frac{1}{3}} - 0.03962\nu^{-1} - 0.3958\nu^{-\frac{5}{3}} + \cdots, \\ j'_{\nu,3} &\sim \nu + 3.8257153\nu^{\frac{1}{3}} + 4.430038\nu^{-\frac{1}{3}} - 0.15018\nu^{-1} - 1.7173\nu^{-\frac{5}{3}} + \cdots, \\ j'_{\nu,4} &\sim \nu + 4.8918203\nu^{\frac{1}{3}} + 7.209635\nu^{-\frac{1}{3}} - 0.32456\nu^{-1} - 4.4671\nu^{-\frac{5}{3}} + \cdots, \\ j'_{\nu,5} &\sim \nu + 5.8513010\nu^{\frac{1}{3}} + 10.296952\nu^{-\frac{1}{3}} - 0.56244\nu^{-1} - 9.0480\nu^{-\frac{5}{3}} + \cdots, \end{aligned} \tag{49}$$

and of $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}Y^\nu(x)]/dx$ are

$$\begin{aligned} \bar{y}'_{\nu,1} &\sim \nu + 1.8210980\nu^{\frac{1}{3}} + 1.077287\nu^{-\frac{1}{3}} - 0.00912\nu^{-1} - 0.1263\nu^{-\frac{5}{3}} + \cdots, \\ \bar{y}'_{\nu,2} &\sim \nu + 3.2328653\nu^{\frac{1}{3}} + 3.181824\nu^{-\frac{1}{3}} - 0.08687\nu^{-1} - 0.9055\nu^{-\frac{5}{3}} + \cdots, \\ \bar{y}'_{\nu,3} &\sim \nu + 4.3751914\nu^{\frac{1}{3}} + 5.776974\nu^{-\frac{1}{3}} - 0.22942\nu^{-1} - 2.8873\nu^{-\frac{5}{3}} + \cdots, \\ \bar{y}'_{\nu,4} &\sim \nu + 5.3823170\nu^{\frac{1}{3}} + 8.718670\nu^{-\frac{1}{3}} - 0.43556\nu^{-1} - 6.5053\nu^{-\frac{5}{3}} + \cdots, \\ \bar{y}_{\nu,5} &\sim \nu + 6.3021240\nu^{\frac{1}{3}} + 11.938832\nu^{-\frac{1}{3}} - 0.70519\nu^{-1} - 12.1392\nu^{-\frac{5}{3}} + \cdots. \end{aligned} \tag{50}$$

We can also make use of the Olver asymptotic expansions (40) and (41) to obtain the value $[\frac{1}{2}\pi\bar{\sigma}'_\nu(t)]^{\frac{1}{2}}\mathcal{C}_{\nu,t}(\bar{\sigma}'_\nu(t))$ of the Riccati–Bessel function at the zero of its derivative. Thus we expand $\mathcal{C}_{\nu,t}(\bar{\sigma}'_\nu(t))$ in a Taylor series about $\nu + \alpha_1\nu^{\frac{1}{3}}$, so that

$$\begin{aligned} \mathcal{C}_{\nu,t}(\bar{\sigma}'_\nu(t)) &= \sum_{m=0}^{\infty} \frac{\epsilon^m}{m!} \mathcal{C}^{(m)}_{\nu,t}(\nu + \alpha_1\nu^{\frac{1}{3}}) \\ &\sim \sum_{m=0}^{\infty} \frac{\epsilon^m}{m!} \Bigg\{ \frac{2^{\frac{1}{3}}}{\nu^{\frac{1}{3}(m+1)}} [(\cos \pi t)\,\mathrm{Ai}(-2^{\frac{1}{3}}\alpha_1) - (\sin \pi t)\,\mathrm{Bi}(-2^{\frac{1}{3}}\alpha_1)] \sum_{s=0}^{\infty} \frac{A_s^m(\alpha_1)}{\nu^{\frac{2}{3}s}} \\ &\quad + \frac{2^{\frac{2}{3}}}{\nu^{\frac{1}{3}(m+1)}} [(\cos \pi t)\,\mathrm{Ai}'(-2^{\frac{1}{3}}\alpha_1) - (\sin \pi t)\,\mathrm{Bi}'(-2^{\frac{1}{3}}\alpha_1)] \sum_{s=0}^{\infty} \frac{B_s^m(\alpha_1)}{\nu^{\frac{2}{3}s}} \Bigg\}, \end{aligned} \tag{51}$$

where

$$\bar{\sigma}'_\nu(t) = \nu + \alpha_1\nu^{\frac{1}{3}} + \epsilon \sim \nu + \alpha_1\nu^{\frac{1}{3}} + \alpha_2\nu^{-\frac{1}{3}} + \alpha_3\nu^{-1} + \alpha_4\nu^{-\frac{5}{3}} + \cdots. \tag{52}$$

The second part of the expansion (51) vanishes by the original choice of α_1 in Eq. (45). The remaining expression can be expanded in descending powers of $\nu^{\frac{2}{3}}$ to give

$$\mathcal{C}_{\nu,t}(\bar{\sigma}'_\nu(t)) \sim \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{\lambda}{\nu^{\frac{1}{3}}} \left(1 + \frac{\theta_1}{\nu^{\frac{2}{3}}} + \frac{\theta_2}{\nu^{\frac{4}{3}}} + \frac{\theta_3}{\nu^2} + \cdots\right) \tag{53}$$

[16] Zeros of the Airy functions may be obtained from *British Association for the Advancement of Science Mathematical Tables, Part-Vol. B, The Airy Integral*, J. C. P. Miller, Ed. (Cambridge University Press, Cambridge, England, 1946).

with

$$\lambda = (\pi/2)^{\frac{1}{2}}2^{\frac{1}{3}}[(\cos \pi t)\,\mathrm{Ai}\,(-2^{\frac{1}{3}}\alpha_1) - (\sin \pi t)\,\mathrm{Bi}\,(-2^{\frac{1}{3}}\alpha_1)], \tag{54}$$

$$\theta_1 = -\tfrac{1}{5}\alpha_1, \quad \theta_2 = -\tfrac{21}{400}\alpha_1^{-1} + \tfrac{9}{350}\alpha_1^2,$$
$$\theta_3 = \tfrac{9}{2000}\alpha_1^{-3} + \tfrac{937}{18000} + \tfrac{89}{15750}\alpha_1^3. \tag{55}$$

The value of the Riccati–Bessel function is

$$(\tfrac{1}{2}\pi\bar{\sigma}_\nu'(t))^{\frac{1}{2}}\mathcal{C}_{\nu,t}(\bar{\sigma}_\nu'(t)) \sim \lambda\nu^{\frac{1}{6}}(1 + \omega_1\nu^{-\frac{2}{3}} + \omega_2\nu^{-\frac{4}{3}} + \omega_3\nu^{-2} + \cdots), \tag{56}$$

where

$$\omega_1 = \tfrac{3}{10}\alpha_1, \quad \omega_2 = \tfrac{9}{400}\alpha_1^{-1} - \tfrac{69}{1400}\alpha_1^2,$$
$$\omega_3 = -\tfrac{9}{8000}\alpha_1^{-3} - \tfrac{781}{36000} - \tfrac{53}{126000}\alpha_1^3. \tag{57}$$

For the Bessel and Neumann forms, the expansions are given by

$$\begin{aligned}
(\tfrac{1}{2}\pi j_{\nu,1}')^{\frac{1}{2}}J_\nu(j_{\nu,1}') &\sim +0.8458430\nu^{\frac{1}{6}}(1 + 0.242585\nu^{-\frac{2}{3}} - 0.00440\nu^{-\frac{4}{3}} - 0.0240\nu^{-2} + \cdots),\\
(\tfrac{1}{2}\pi j_{\nu,2}')^{\frac{1}{2}}J_\nu(j_{\nu,2}') &\sim -0.6616576\nu^{\frac{1}{6}}(1 + 0.773429\nu^{-\frac{2}{3}} - 0.31885\nu^{-\frac{4}{3}} - 0.0290\nu^{-2} + \cdots),\\
(\tfrac{1}{2}\pi j_{\nu,3}')^{\frac{1}{2}}J_\nu(j_{\nu,3}') &\sim +0.6006911\nu^{\frac{1}{6}}(1 + 1.147715\nu^{-\frac{2}{3}} - 0.71547\nu^{-\frac{4}{3}} - 0.0453\nu^{-2} + \cdots),
\end{aligned} \tag{58}$$

$$\begin{aligned}
(\tfrac{1}{2}\pi y_{\nu,1}')^{\frac{1}{2}}Y_\nu(y_{\nu,1}') &\sim +0.7183921\nu^{\frac{1}{6}}(1 + 0.546329\nu^{-\frac{2}{3}} - 0.15110\nu^{-\frac{4}{3}} - 0.0244\nu^{-2} + \cdots),\\
(\tfrac{1}{2}\pi y_{\nu,2}')^{\frac{1}{2}}Y_\nu(y_{\nu,2}') &\sim -0.6261400\nu^{\frac{1}{6}}(1 + 0.969860\nu^{-\frac{2}{3}} - 0.50815\nu^{-\frac{4}{3}} - 0.0359\nu^{-2} + \cdots),\\
(\tfrac{1}{2}\pi y_{\nu,3}')^{\frac{1}{2}}Y_\nu(y_{\nu,3}') &\sim +0.5810516\nu^{\frac{1}{6}}(1 + 1.312557\nu^{-\frac{2}{3}} - 0.93830\nu^{-\frac{4}{3}} - 0.0569\nu^{-2} + \cdots).
\end{aligned} \tag{59}$$

In Sec. 2, we are interested in the values of the second derivative of the Riccati–Bessel functions at the zeros $\bar{\sigma}_\nu'(t)$ of the first derivatives. These values may be found from the expansions given above for $(\frac{1}{2}\pi\bar{\sigma}_\nu'(t))^{\frac{1}{2}}\mathcal{C}_{\nu,t}(\bar{\sigma}_\nu'(t))$ and the differential equation for the Riccati–Bessel functions

$$\frac{d^2}{dx^2}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}\mathcal{C}_{\nu,t}(x)\right] = -\left(1 - \frac{4\nu^2 - 1}{4x^2}\right)\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}\mathcal{C}_{\nu,t}(x). \tag{60}$$

Alternatively, one can expand the second derivative directly and again employ the Olver asymptotic expansions (40) and (41). We find

$$\frac{d^2}{dx^2}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}}\mathcal{C}_{\nu,t}(x)\right]_{x=\bar{\sigma}_\nu(t)} \sim \frac{\lambda}{\nu^{\frac{1}{2}}}\left(\delta_0 + \frac{\delta_1}{\nu^{\frac{2}{3}}} + \frac{\delta_2}{\nu^{\frac{4}{3}}} + \cdots\right), \tag{61}$$

where

$$\delta_0 = -2\alpha_1, \quad \delta_1 = -\tfrac{3}{10}\alpha_1^{-1} + \tfrac{9}{5}\alpha_1^2,$$
$$\delta_2 = \tfrac{9}{400}\alpha_1^{-3} + \tfrac{99}{200} - \tfrac{963}{700}\alpha_1^3. \tag{62}$$

2. ZEROS OF THE CROSS PRODUCTS OF RICCATI-BESSEL FUNCTIONS AND OF DERIVATIVES

Zeros of the Cross Product of Bessel Functions

The frequencies for transverse electric normal modes in the region between two spherical conducting shells are given by the zeros of the function

$$\frac{xj_l(x)}{xy_l(x)} - \frac{xj_l(Kx)}{xy_l(Kx)} \tag{63}$$

and, hence, these were the zeros of original interest to the author. However, since these zeros are identical with those for

$$\frac{J_\nu(x)}{Y_\nu(x)} - \frac{J_\nu(Kx)}{Y_\nu(Kx)}, \quad \nu = l + \tfrac{1}{2}, \tag{64}$$

we will again phrase our results in terms of the more familiar cylindrical Bessel functions $J_\nu(x)$, $Y_\nu(x)$. The zeros $x_{\nu,K,s}$ of (64) have been investigated by Kalähne,[4] and more recently some of the zeros for $\nu = l + \frac{1}{2}$ have been computed by Chandrasekhar and Elbert.[17] After reviewing some of Kalähne's results, we present derivations for asymptotic expansions of the zeros for large ν, and for large and small K. These expansions do not seem to have been presented previously in the literature. In some cases they confirm and in some contradict Kalähne's conjectures about the behavior of the zeros. Graphs showing the behavior are provided for $\nu = l + \frac{1}{2}$ with l integral.

For real ν and $K > 1$, the function in (64) has an infinite number of zeros all of which are real.[18] The positive zeros $x_{\nu,K,s}$ are simple. The zeros are interlaced in adjacent order in qualitatively the same fashion as the zeros of the cylinder functions $\mathcal{C}_{\nu,t}(x)$. Many of the qualitative features of the dependence of the zeros $x_{\nu,K,s}$ on ν and s can be seen from Fig. 3,

[17] S. Chandrasekhar and D. Elbert, Proc. Cambridge Phil. Soc. **49**, 446 (1953).

[18] A. Gray and S. B. Mathews, *A Treatise on Bessel Functions* (Macmillan and Co., Ltd., London, 1922), 2nd Ed., p. 82. Also Ref. 1, p. 507.

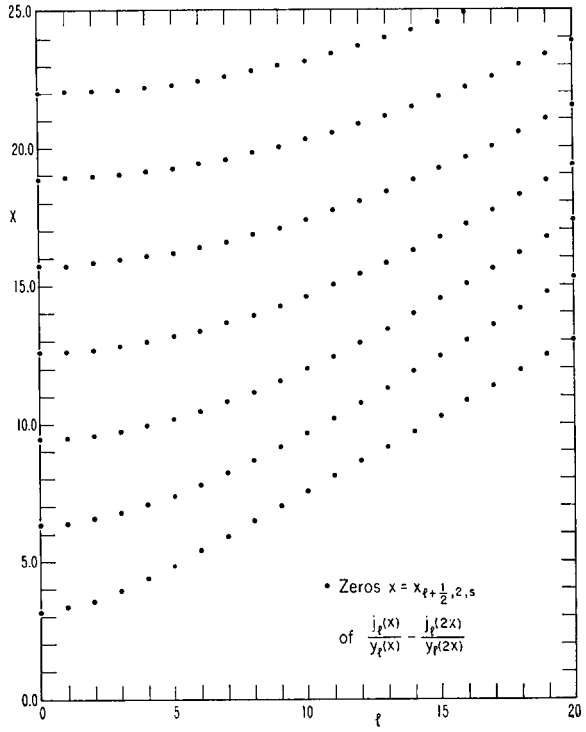


FIG. 3. Zeros of $(j_l(x)/y_l(x)) - (j_l(2x)/y_l(2x))$.

showing the small zeros $x_{l+\frac{1}{2},2,s}$ for $l = 0(1)20$. This figure also should be compared with that for the Bessel function zeros $j_{l+\frac{1}{2},s}$ in Fig. 2.

All the essentials of the behavior of the zeros can be understood by superimposing the graphs of $J_\nu(x)/Y_\nu(x)$ and $J_\nu(Kx)/Y_\nu(Kx)$ as in Fig. 4 for $\nu = 5\frac{1}{2}$. The pattern can be thought of as the same curve with two different scales for the abscissa governed by the parameter K. We return repeatedly to this notion when discussing the expected qualitative behavior of the zeros.

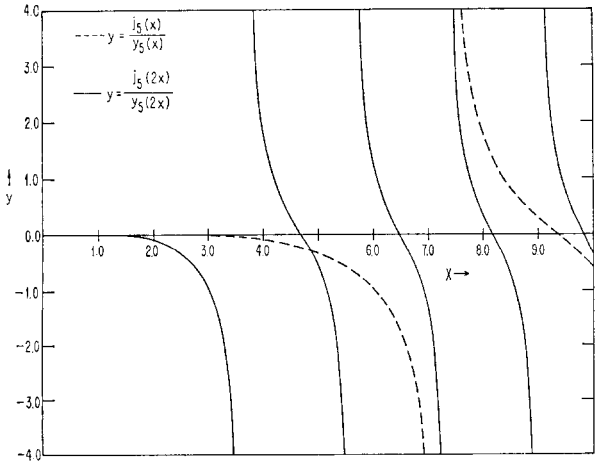


FIG. 4. Functions $j_5(x)/y_5(x)$ and $j_5(2x)/y_5(2x)$. The intersections of the curves give the zeros $x_{5\frac{1}{2},2,s}$ of $(j_5(x)/y_5(x)) - (j_5(2x)/y_5(2x))$.

Expansions of the Zeros for Large Numbers

The expansion for the large zeros $x_{\nu,K,s}$ of (64) for fixed ν was carried out by McMahon on the same paper[3] in which he developed that for the zeros of $J_\nu(x)$. We repeat his result here:

$$x_{\nu,K,s} \sim \beta + \frac{p}{\beta} + \frac{q-p^2}{\beta^3} + \frac{r-4pq+2p^3}{\beta^5} + \cdots, \tag{65}$$

where

$$\beta = \pi s/(K-1), \quad \mu = 4\nu^2,$$
$$p = \frac{\mu-1}{8K}, \quad q = \frac{(\mu-1)(\mu-25)(K^3-1)}{6(4K)^3(K-1)},$$
$$r = \frac{(\mu-1)(\mu^2-114\mu+1073)(K^5-1)}{5(4K)^5(K-1)}. \tag{66}$$

Figure 5 for $\nu = 5\frac{1}{2}$ shows the approach of the large zeros $x_{\nu,K,s}$ to multiples of π for increasing s, and indicates that as K becomes large, the approach to this limit becomes progressively slower, as is indicated by (65).

Limit as $K \to 1$

The form of the McMahon expansion (65) and the appearance of Fig. 5 suggests the behavior of the zeros in the limit as $K \to 1$. We note that all the expansion coefficients (66) go to constants as $K \to 1$, since all involve $(K^n - 1)/(K-1)$. Now $\beta \propto (K-1)^{-1}$ and hence becomes increasingly large as $K \to 1$. Thus *all* of the zeros become large in magnitude as $K \to 1$, and all approach $\pi/(K-1)$ according to the expansion (65). The first term may be found directly by substituting directly into (64) the asymptotic

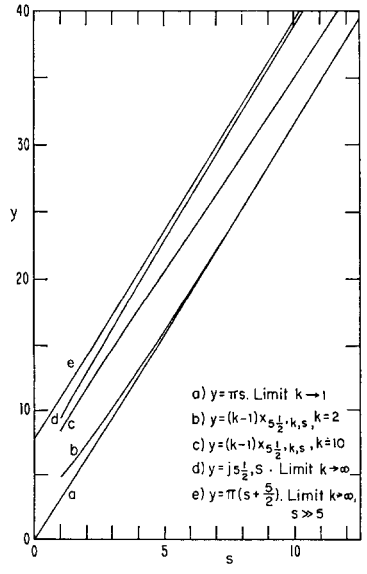


FIG. 5. Zeros of $(j_5(x)/y_5(x)) - (j_5(Kx)/y_5(Kx))$ for $K = 2, 10$; $K \to 1, \infty$. The zeros $x_{5\frac{1}{2},K,s}$ for $s = 1, 2, \cdots, 12$ are given for the values of the parameter $K = 2$, 10 and limits $K \to 1$, $K \to \infty$. The straight line $y = \pi s$ gives the $K \to 1$ limit of $(K-1)x_{5\frac{1}{2},K,s}$, and also the $s \to \infty$ limit for any finite K. The line $y = \pi(s + \frac{5}{2})$ gives the $K \to \infty$ limit of $(K-1)x_{5\frac{1}{2},K,s}$ for $s \gg 5$. The $K \to \infty$ limit points of $(K-1) \times x_{5\frac{1}{2},K,s}$ are the zeros $j_{5\frac{1}{2},s}$ of $j_5(x)$.

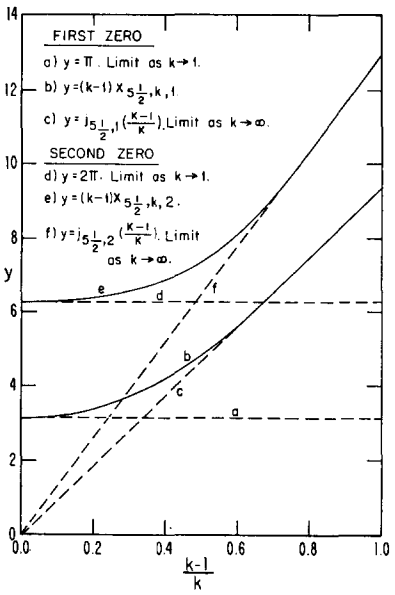


FIG. 6. First two zeros of $(j_5(x)/y_5(x)) - (j_5(Kx)/y_5(Kx))$ as a function of K. The dependence on the parameter K of the first two zeros $x_{\nu,K,s}$ of (64) for $\nu = 5\frac{1}{2}$ is indicated by the solid curves b and e. The broken curves indicate the limiting behavior as $K \to 1$ and $K \to \infty$. The values of the zeros $j_{5\frac{1}{2},s}$ of $j_5(x)$ are $j_{5\frac{1}{2},1} = 9.355812111043$, $j_{5\frac{1}{2},2} = 12.96653017277$.

forms holding for large x:

$$J_\nu(x) \sim (2/\pi x)^{\frac{1}{2}} \sin [x - \tfrac{1}{2}\pi(\nu - \tfrac{1}{2})],$$
$$Y_\nu(x) \sim -(2/\pi x)^{\frac{1}{2}} \cos [x - \tfrac{1}{2}\pi(\nu - \tfrac{1}{2})]. \quad (67)$$

We arrive at the requirement for a zero at x:

$$\tan [x - \tfrac{1}{2}\pi(\nu - \tfrac{1}{2})] \sim \tan [Kx - \tfrac{1}{2}\pi(\nu - \tfrac{1}{2})], \quad (68)$$

which requires

$$Kx - \tfrac{1}{2}\pi(\nu - \tfrac{1}{2}) \sim \pi s + x - \tfrac{1}{2}\pi(\nu - \tfrac{1}{2})$$
$$\text{or} \quad x \sim \pi s/(K - 1), \quad (69)$$

as found above.

Figures 5 and 6 indicate the behavior of the low zeros for $\nu = 5\frac{1}{2}$. It is clearly convenient to plot $(K - 1)x_{\nu,K,s}$ rather than simply $x_{\nu,K,s}$, so that as $K \to 1$ the values become multiples of π.

Limit as $K \to \infty$

Juxtaposition of the graphs for $J_\nu(x)/Y_\nu(x)$ and $J_\nu(Kx)/Y_\nu(Kx)$ allows one to decide on the qualitative features of $x_{\nu,K,s}$ in two more asymptotic limits; for fixed ν and $K \to \infty$ or for fixed K and $\nu \to \infty$, the low zeros become the zeros $j_{\nu,s}/K$ of $J_\nu(Kx)/Y_\nu(Kx)$. We now consider these limits separately in some detail.

In order to obtain the asymptotic expansion for $x_{\nu,K,s}$ as $K \to \infty$, we expand $J_\nu(Kx)/Y_\nu(Kx)$ with $x = x_{\nu,K,s} = (j_{\nu,s}/K) + \epsilon$ in a Taylor series about $j_{\nu,s}/K$, and expand $J_\nu(x)/Y_\nu(x)$ in ascending powers for small argument $x = x_{\nu,K,s}$. Thus the condition for a zero of (64) is

$$\epsilon K \frac{d}{dz}\left(\frac{J_\nu(z)}{Y_\nu(z)}\right)_{z=j_{\nu,s}} + \frac{\epsilon^2}{2!} K^2 \frac{d^2}{dz^2}\left(\frac{J_\nu(z)}{Y_\nu(z)}\right)_{z=j_{\nu,s}} + \cdots = \frac{J_\nu((j_{\nu,s}/K) + \epsilon)}{Y_\nu((j_{\nu,s}/K) + \epsilon)}, \quad (70)$$

where

$$J_\nu\left(\frac{j_{\nu,s}}{K} + \epsilon\right) = \left[\frac{1}{2}\left(\frac{j_{\nu,s}}{K} + \epsilon\right)\right]^\nu \times \sum_{r=0}^{\infty} \frac{(-1)^r[\frac{1}{2}((j_{\nu,s}/K) + \epsilon)]^{2r}}{r!\,(\nu + r)!}$$
$$\sim \left(\frac{j_{\nu,s}}{2K}\right)^\nu \frac{1}{\Gamma(\nu + 1)}, \quad (71)$$

$$Y_\nu\left(\frac{j_{\nu,s}}{K} + \epsilon\right) = -\left[\frac{1}{2}\left(\frac{j_{\nu,s}}{K} + \epsilon\right)\right]^{-\nu} \times \sum_{r=0}^{r=\nu-1} \frac{(\nu - r - 1)!}{r!}\left[\frac{1}{2}\left(\frac{j_{\nu,s}}{K} + \epsilon\right)\right]^{2r} + \frac{2}{\pi} \ln \left[\frac{1}{2}\left(\frac{j_{\nu,s}}{K} + \epsilon\right)\right] J_\nu\left(\frac{j_{\nu,s}}{K} + \epsilon\right) - \frac{[\frac{1}{2}((j_{\nu,s}/K) + \epsilon)]^\nu}{\pi} \times \sum_{r=0}^{\infty} \{\psi(r + 1) + \psi(\nu + r + 1)\} \times \frac{(-1)^r[\frac{1}{2}((j_{\nu,s}/K) + \epsilon)]^{2r}}{r!\,(\nu + K)!}$$
$$\sim \frac{2}{\pi} \ln \left(\frac{j_{\nu,s}}{K}\right), \qquad \nu = 0,$$
$$\sim -\frac{1}{\pi}\Gamma(\nu)\left(\frac{j_{\nu,s}}{2K}\right)^{-\nu}, \quad \nu > 0. \quad (72)$$

The first approximation for ϵ may be found by ignoring higher powers of ϵ on both sides of Eq. (70). Dividing through by

$$K \frac{d}{dz}\left(\frac{J_\nu(z)}{Y_\nu(z)}\right)_{z=j_{\nu,s}} = -\frac{\pi}{2} K j_{\nu,s}(J'_\nu(j_{\nu,s}))^2, \quad (73)$$

we have

$$\epsilon \sim \frac{-1}{Kj_{0,s}(J'_0(j_{0,s}))^2 \ln (K/j_{0,s})}, \qquad \nu = 0,$$
$$\sim \frac{2(j_{\nu,s}/2K)^{2\nu}}{Kj_{\nu,s}(J'_\nu(j_{\nu,s}))^2\Gamma(\nu)\Gamma(\nu + 1)}, \quad \nu > 0. \quad (74)$$

In obtaining Eq. (73), we have employed the Wronskian relation for the Bessel functions

$$J_\nu(z)Y'_\nu(z) - Y_\nu(z)J'_\nu(z) = 2/\pi z. \quad (75)$$

In every case, $\epsilon = o(1/K)$, going to zero faster than $1/K$, so that, as conjectured, $Kx_{\nu,K,s} \to j_{\nu,s}$ as $K \to \infty$. The full functional dependence of ϵ on K must be found by comparing both sides of Eq. (70).

The analysis for $\nu = l + \frac{1}{2}$, l integral, is simpler

algebraically since both $j_l(x)$ and $y_l(x)$ allow expansions in ascending powers of x:

$$j_l(x) = \frac{x^l}{1\cdot 3\cdot 5\cdots(2l+1)}\left\{1 - \frac{\frac{1}{2}x^2}{1!\,(2l+3)} + \frac{(\frac{1}{2}x^2)^2}{2!\,(2l+3)(2l+5)} - \cdots\right\}, \quad (76)$$

$$y_l(x) = \frac{-1\cdot 3\cdot 5\cdots(2l-1)}{x^{l+1}}\left\{1 - \frac{\frac{1}{2}x^2}{1!\,(1-2l)} + \frac{(\frac{1}{2}x^2)^2}{2!\,(1-2l)(3-2l)} - \cdots\right\}. \quad (77)$$

Using these expressions in place of Eqs. (71) and (72), we find ϵ allows an expansion in descending powers of K starting at $K^{-(2l+2)}$ so that

$$x_{l+\frac{1}{2},K,s} \sim \frac{j_{l+\frac{1}{2},s}}{K} - \frac{(j_{l+\frac{1}{2},s})^{2l-1}}{K^{2l+2}(j_l'(j_{l+\frac{1}{2},s}))^2} \cdot \frac{(2l+1)}{(1\cdot 3\cdot 5\cdots(2l+1))^2} + O(K^{-2l-4}). \quad (78)$$

When ν becomes large, we can employ the ν asymptotic expansions of Eq. (25) for the Bessel zeros $j_{\nu,s}$, and of Eq. (26) for $J_\nu'(j_{\nu,s})$, and hence may write $x_{\nu,K,s}$ entirely in terms of fractional powers of ν with coefficients given explicitly on Sec. 1.

The dependence of the small zeros $x_{\nu,K,s}$ of (64) for $\nu = 5\frac{1}{2}$ is shown in Figs. 5 and 6. For all $\nu > \frac{1}{2}$ as $K \to \infty$, the zeros approach straight lines $y = j_{\nu,s}[(K-1)/K]$ corresponding to the asymptotic behavior of the zeros as $x_{\nu,K,s} \sim j_{\nu,s}/K$. We remark that Kalähne has plotted a comparable graph[19] with a different abscissa and hence the asymptotic form as $K \to \infty$ is more complicated, and indeed even erroneous in those (dashed) curves which Kalähne drew by conjecture without numerical computations.

Limit as $\nu \to \infty$

For any fixed $K > 1$, as the order ν of the Bessel functions increases, the zeros $x_{\nu,K,s}$ again become the zeros $j_{\nu,s}/K$ of $J_\nu(Kx)/Y_\nu(Kx)$. This follows because the initial flat region of $J_\nu(x)/Y_\nu(x)$ seen in Fig. 4 becomes proportionally longer compared to the distance between the zeros. Indeed, the distance to the first zero is $O(\nu^{\frac{1}{3}})$, so that for increasingly large ν, the function $J_\nu(Kx)/Y_\nu(Kx)$ crosses the graph of $J_\nu(x)/Y_\nu(x)$ an increasing number of times in this region where the latter's value becomes progressively smaller.

The asymptotic form for the zeros may be obtained in much the same way exploited in the previous section. We expand $J_\nu(Kx)/Y_\nu(Kx)$, $x = x_{\nu,K,s} = (j_{\nu,s}/K) + \epsilon$ in a Taylor series about $j_{\nu,s}/K$, while for $J_\nu(x)/Y_\nu(x)$ the Debye asymptotic expansions are suitable. Thus the requirement for a zero of (64) at $(j_{\nu,s}/K) + \epsilon$ is

$$\epsilon\frac{d}{dx}\left(\frac{J_\nu(Kx)}{Y_\nu(Kx)}\right)_{x=j_{\nu,s}/K} + \epsilon^2\frac{d^2}{dx^2}\left(\frac{J_\nu(Kx)}{Y_\nu(Kx)}\right)_{x=j_{\nu,s}/K} + \cdots = \frac{J_\nu((j_{\nu,s}/K)+\epsilon)}{Y_\nu((j_{\nu,s}/K)+\epsilon)}, \quad (79)$$

with

$$J_\nu\left(\frac{j_{\nu,s}}{K} + \epsilon\right) \sim \frac{\exp[\nu(\tanh\beta - \beta)]}{(2\pi\nu\tanh\beta)^{\frac{1}{2}}} \times \left\{1 + \sum_{r=1}^{\infty}\frac{u_r(\coth\beta)}{\nu^r}\right\}, \quad (80)$$

$$Y_\nu\left(\frac{j_{\nu,s}}{K} + \epsilon\right) \sim \frac{-\exp[-\nu(\tanh\beta - \beta)]}{(\frac{1}{2}\pi\nu\tanh\beta)^{\frac{1}{2}}} \times \left\{1 + \sum_{r=1}^{\infty}(-1)^r\frac{u_r(\coth\beta)}{\nu^r}\right\}, \quad (81)$$

where

$$\operatorname{sech}\beta = \frac{j_{\nu,s}}{\nu K} + \frac{\epsilon}{\nu} \sim \frac{1}{K}(1 + \alpha_1\nu^{-\frac{2}{3}} + \alpha_2\nu^{-\frac{4}{3}} + \cdots) + \frac{\epsilon}{\nu} \quad (82)$$

and the $u_r(t)$ are polynomials

$$u_1(t) = \tfrac{1}{24}(3t - 5t^3),$$
$$u_2(t) = \tfrac{1}{1152}(81t^2 - 462t^4 + 385t^6), \cdots. \quad (83)$$

We note that inasmuch as $K > 1$ is required, there is some ν_0 above which $j_{\nu,s}/\nu K < 1$, and we can find a real number $\beta_\nu > 0$ such that

$$\operatorname{sech}\beta_\nu = \frac{1}{K}\frac{j_{\nu,s}}{\nu}. \quad (84)$$

Since $\tanh\beta_\nu - \beta_\nu < 0$ for $\beta_\nu > 0$, the first approximation for ϵ is exponentially small in ν:

$$\epsilon \sim \frac{\pi\exp[2\nu(\tanh\beta_\nu - \beta_\nu)]}{Kj_{\nu,s}(J_\nu'(j_{\nu,s}))^2}. \quad (85)$$

We have again used Eq. (73) to rewrite

$$\frac{d}{dx}\left(\frac{J_\nu(Kx)}{Y_\nu(Kx)}\right)_{x=j_{\nu,s}/K}.$$

The full asymptotic expansion should be obtained by using asymptotic expansions (25) and (26) for $j_{\nu,s}$ and $J_\nu'(j_{\nu,s})$ to obtain those for all the coefficients of ϵ on the left-hand side of Eq. (79)—which is possible since the Bessel functions satisfy a second-order

[19] See Ref. 4, p. 78, Fig. 1, and also Kalähne's conjectures in the text regarding the asymptotic behavior.

differential equation—and then comparing terms in $\exp[2\nu(\tanh\beta_\nu - \beta_\nu)]$ times fractional powers of ν^{-1} on both sides of Eq. (79).

Figure 7 shows the approach of the low zeros $x_{l+\frac{1}{2},K,s}$ to $j_{l+\frac{1}{2},s}/K$ for $K = 2$, $s = 1, 2$ as l increases from 0 to 10. Note that the ordinate has been chosen as $y = Kx_{l+\frac{1}{2},K,s}$ so that the normalization is different from that of Figs. 3, 5, and 6. For given ν and large s, or for given ν and $K \to 1$, we saw that the zeros $x_{\nu,K,s} \sim \pi s/(K-1)$, and it was thus convenient to plot $(K-1)x_{\nu,K,s}$. However, for given ν and large K or for given K and large ν, the zeros $x_{\nu,K,s} \sim j_{\nu,s}/K$. Thus to illustrate these limits it is most convenient to plot $Kx_{\nu,K,s}$, as is actually done only in Fig. 7 for $\nu \to \infty$. The limit for large K was illustrated by approach to the straight lines of Fig. 6, involving the $(K-1)x_{\nu,K,s}$ normalization. No single graph seems to provide easily the information for all asymptotic limits.

Zeros of the Cross Product of the Derivatives of the Riccati-Bessel Functions

Corresponding to (64) for the Riccati-Bessel functions, or Bessel functions equally well, we wish finally to consider the zeros of

$$\frac{\dfrac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}} J_\nu(x)\right]}{\dfrac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}} Y_\nu(x)\right]} - \frac{\dfrac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}} J_\nu(Kx)\right]}{\dfrac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}} Y_\nu(Kx)\right]}, \tag{86}$$

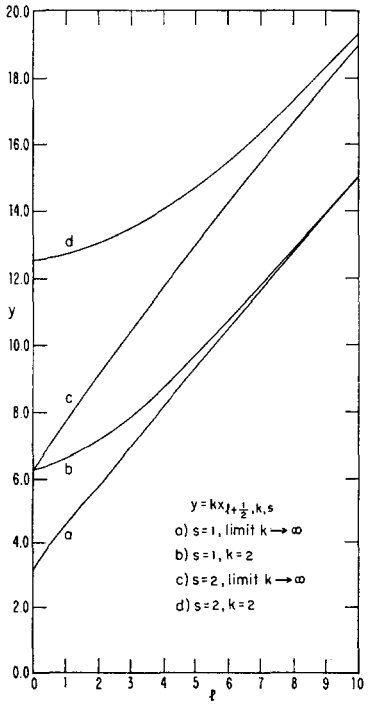


FIG. 7. First two zeros of

$$(j_l(x)/y_l(x)) - (j_l(Kx)/y_l(Kx))$$

for $0 \leq l \leq 10$, $K = 2$, $K \to \infty$. The first two zeros $x_{l+\frac{1}{2},K,s}$ of (64) for small values of $\nu = l + \frac{1}{2}$ are given as $Kx_{l+\frac{1}{2},K,s}$ for $K = 2$, $K \to \infty$. As l increases, curves for finite K approach the results $j_{l+\frac{1}{2},s}$ for the $K \to \infty$ limit.

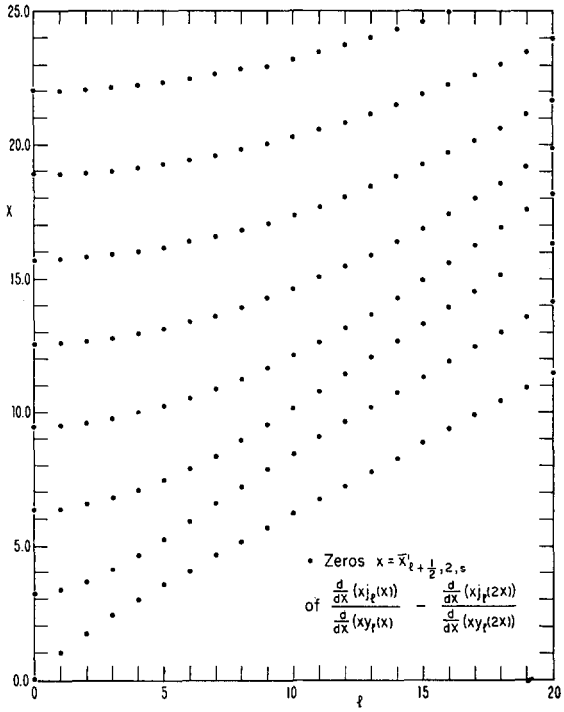


FIG. 8. Zeros of

$$\frac{d(xj_l(x))/dx}{d(xy_l(x))/dx} - \frac{d(xj_l(2x))/dx}{d(xy_l(2x))/dx}.$$

involving the derivatives of the Riccati-Bessel functions. This can also be written in terms of spherical Bessel functions as the function

$$\frac{\dfrac{d}{dx}(xj_l(x))}{\dfrac{d}{dx}(xy_l(x))} - \frac{\dfrac{d}{dx}(xj_l(Kx))}{\dfrac{d}{dx}(xy_l(Kx))} \tag{87}$$

which arises for the transverse magnetic normal modes in the region between two spherical conducting shells. We find that the behavior of the zeros $\bar{x}'_{\nu,K,s}$, as seen for example in Fig. 8 for $K = 2$, is roughly analogous to that of the $x_{\nu,K,s}$ which were considered above, except for the somewhat irregular behavior of the first zero.

Figure 9 shows the graphs of

$$\frac{\dfrac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}} J_\nu(x)\right]}{\dfrac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}} J_\nu(x)\right]} \quad \text{and} \quad \frac{\dfrac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}} J_\nu(Kx)\right]}{\dfrac{d}{dx}\left[\left(\frac{\pi x}{2}\right)^{\frac{1}{2}} Y_\nu(Kx)\right]}$$

for $K = 2$, $\nu = 5\frac{1}{2}$, plotted on the same axis. The abscissas of the intersection points of the graphs correspond to the desired zeros. We note that for $\nu > \frac{1}{2}$ here, in contrast to the case for (64), because the first positive zero of $d[(\frac{1}{2}\pi x)^{\frac{1}{2}} J_\nu(x)]/dx$ lies below

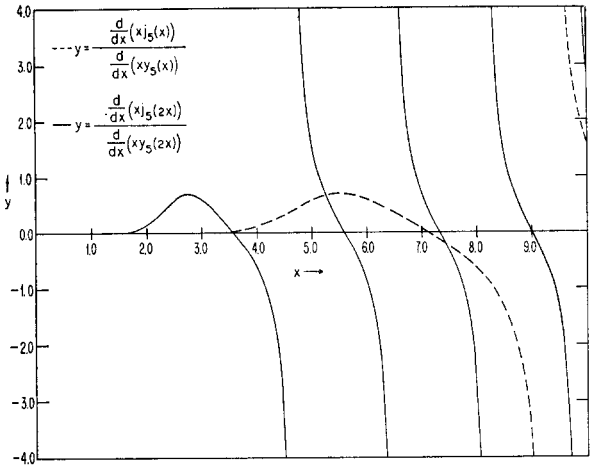


FIG. 9. Functions

$$\frac{d(xj_5(x))/dx}{d(xy_5(x))/dx} \quad \text{and} \quad \frac{d(xj_5(2x))/dx}{d(xy_5(2x))/dx}.$$

The abscissas of the points of intersection are the zeros $\bar{x}'_{5\frac{1}{2},2,s}$ of (86).

the first positive zero of $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}Y_\nu(x)]/dx$, the lowest zero of (86) occurs below the first infinity of

$$\frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(Kx)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(Kx)\right]}.$$

Otherwise Figs. 9 and 4 look remarkably similar. The infinite numbers of zeros and interlacing patterns for orders ν differing by one unit are again expected, and are illustrated in Fig. 8 for the case $K = 2$.

Expansions for Large Number of the Zero

The expansion for the large number s of the zero can again be derived after the manner of McMahon's work. Writing the Bessel functions in terms of trigonometric functions and a series in descending powers of x as in Eqs. (30) and (31), and noting that

$$\frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x)\right]}$$

$$= \frac{-\tan\left[x - \dfrac{\pi}{2}(\nu + \tfrac{1}{2})\right] + \left(\dfrac{\psi_\nu(x) + \varphi'_\nu(x)}{\varphi_\nu(x) - \psi'_\nu(x)}\right)}{1 + \tan\left[x - \dfrac{\pi}{2}(\nu + \tfrac{1}{2})\right]\left(\dfrac{\psi_\nu(x) + \varphi'_\nu(x)}{\varphi_\nu(x) - \psi'_\nu(x)}\right)}$$

$$= \tan\left[-x + \frac{\pi}{2}(\nu + \tfrac{1}{2}) + \arctan\left(\frac{\psi_\nu(x) + \varphi'_\nu(x)}{\varphi_\nu(x) - \psi'_\nu(x)}\right)\right], \tag{88}$$

we see that the condition for a zero $x = \bar{x}'_{\nu,K,s}$ of (86) is

$$-x + \frac{\pi}{2}(\nu + \tfrac{1}{2}) + \arctan\left(\frac{\psi_\nu(x) + \varphi'_\nu(x)}{\varphi_\nu(x) - \psi'_\nu(x)}\right)$$

$$= \pi(s-1) - Kx + \frac{\pi}{2}(\nu + \tfrac{1}{2})$$

$$+ \arctan\left(\frac{\psi_\nu(Kx) + \varphi'_\nu(Kx)}{\varphi_\nu(Kx) - \psi'_\nu(Kx)}\right), \tag{89}$$

where s is an integer. We have introduced the notation $s - 1$ so that (89) gives the sth positive zero. Expanding the arctangent functions in inverse powers of x under the assumption that the arguments are small as in Eq. (37), and then applying Lagrange's theorem to obtain an expansion in inverse powers of $\beta = \pi(s-1)/(K-1)$, we find

$$\bar{x}'_{\nu,K,s} \sim \beta + \frac{p}{\beta} + \frac{q - p^2}{\beta^3} + \frac{r - 4pq + 2p^3}{\beta^5} + \cdots, \tag{90}$$

where p, q, r are related to the coefficients of Eq. (37) by factors of K, so that $\mu = 4\nu^2$,

$$p = \frac{\mu - 1}{8K}, \quad q = \frac{(\mu-1)(\mu+23)(K^3-1)}{6(4K)^3(K-1)},$$

$$r = \frac{(\mu-1)(\mu^2+126\mu-1087)(K^5-1)}{5(4K)^5(K-1)}. \tag{91}$$

Thus for fixed order ν, the large zeros become $\bar{x}'_{\nu,K,s} \sim \pi(s-1)/(K-1)$. Note that if we replace $s - 1$ by s, this is the same form found for the zeros $x_{\nu,K,s}$ of (64). The large zeros of $x_{\nu,K,s}$ of (64) and $\bar{x}'_{\nu,K,s}$ of (86) go asymptotically to the same values rather than to values midway between zeros of the other function as was found for the pair

$$(\tfrac{1}{2}\pi x)^{\frac{1}{2}}C_{\nu,t}(x), \quad d[(\tfrac{1}{2}\pi x)^{\frac{1}{2}}C_{\nu,t}(x)]/dx,$$

which we consider in Sec. 1. Also, we notice that the first correction terms of Eqs. (65) and (90) are identical.

Limit as $K \to 1$

In the limit as the parameter $K \to 1$ for fixed order ν, we may essentially repeat the same arguments given for the previous case of the zeros $x_{\nu,K,s}$; all the zeros $\bar{x}'_{\nu,K,s}$ except the first become large, and the expansion in terms of Eq. (90) becomes valid for all $\bar{x}'_{\nu,K,s}$ for $s > 1$. The first zero $\bar{x}'_{\nu,K,1}$, however, remains finite, and for $\nu > \frac{1}{2}$ becomes the first maximum of

$$\frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x)\right]},$$

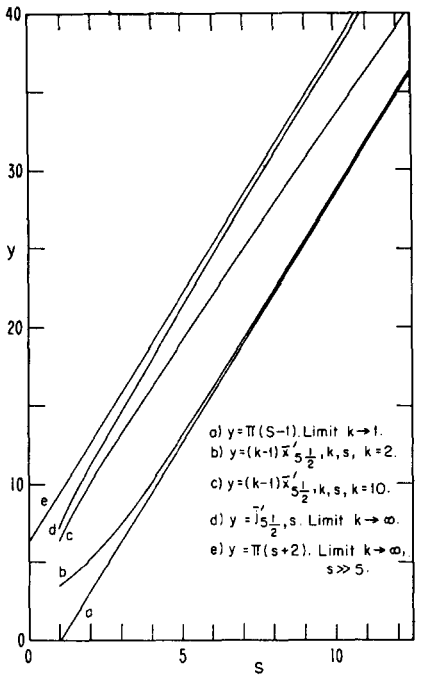


FIG. 10. Zeros of $\dfrac{d(xj_5(x))/dx}{d(xy_5(x))/dx} - \dfrac{d(xj_5(2x))/dx}{d(xy_5(2x))/dx}$, for $K = 2, 10$; $K \to 1, \infty$. The zeros $\bar{x}'_{5\frac{1}{2},K,s}$ for $s = 1, 2, \cdots, 12$ are given for the values of the parameter $K = 2$, 10, and in the limits $K \to 1$, $K \to \infty$. The curve $y = \pi(s-1)$ gives the $K \to 1$ limit of $(K-1)\bar{x}'_{5\frac{1}{2},K,s}$, and also the $s \to \infty$ limit for any finite K. The $K \to \infty$ limit of $(K-1)\bar{x}'_{5\frac{1}{2},K,s}$ are the zeros $\bar{j}'_{5\frac{1}{2},s}$ for $d(xj_5(x))/dx$. The curve $y = \pi(s+2)$ gives the $K\infty \to$ limit of $(K-1)\bar{x}_{5,K,s}$ for $s \gg 5$.

seen for example in Fig. 9. As $\nu \to \frac{1}{2}$, this maximum migrates to the origin, becoming $\bar{x}'_{\nu,K,1} = 0$ for $0 \leq \nu \leq \frac{1}{2}$. See also Fig. 12 in this connection. Alternatively, if we plot $(K-1)\bar{x}'_{\nu,K,s}$ as in Fig. 10, then for $K \to 1$, $(K-1)\bar{x}'_{\nu,K,s} \to \pi(s-1)$ so that the first zero goes to $(K-1)\bar{x}'_{\nu,K,1} \to 0$ and all higher zeros become multiples of π.

Limit as $K \to \infty$

In the antithetical case $K \to \infty$, the limit of $\bar{x}'_{\nu,K,s}$ for ν fixed can be seen from Fig. 9 to present essentially the same behavior as for $x_{\nu,K,s}$ except for small values of ν. Thus,

$$\frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}} J_\nu(x)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}} Y_\nu(x)\right]} \to 0 \tag{92}$$

as $x \to 0$, $\nu \neq \frac{1}{2}$, and the zeros of $\bar{x}'_{\nu,K,s}$ become those $\bar{j}'_{\nu,s}/K$ of $d[(\frac{1}{2}\pi x)^{\frac{1}{2}} J_\nu(x)]/dx$ considered in the second part of Sec. 1.

We expand the terms of (86) depending explicitly on K about $\bar{j}'_{\nu,s}/K$, while expanding the term not containing K about zero in ascending powers of $x = (\bar{j}'_{\nu,s}/K) + \epsilon$. Thus at a zero $\bar{x}'_{\nu,K,s} = (\bar{j}'_{\nu,s}/K) + \epsilon$, we have

$$\epsilon K \frac{d}{dz}\left\{\frac{\dfrac{d}{dz}\left[\left(\dfrac{\pi z}{2}\right)^{\frac{1}{2}} J_\nu(z)\right]}{\dfrac{d}{dz}\left[\left(\dfrac{\pi z}{2}\right)^{\frac{1}{2}} Y_\nu(z)\right]}\right\}_{z=\bar{j}_{\nu,s}'} + \frac{\epsilon^2 K^2}{2!}\frac{d^2}{dz^2}\left\{\frac{\dfrac{d}{dz}\left[\left(\dfrac{\pi z}{2}\right)^{\frac{1}{2}} J_\nu(z)\right]}{\dfrac{d}{dz}\left[\left(\dfrac{\pi z}{2}\right)^{\frac{1}{2}} Y_\nu(z)\right]}\right\}_{z=\bar{j}_{\nu,s}'} + \cdots$$

$$= \left\{\frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}} J_\nu(x)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}} Y_\nu(x)\right]}\right\}_{x=(\bar{j}_{\nu,s}'/K)+\epsilon}. \tag{93}$$

The expressions (71) and (72) may be substituted into the right-hand side of Eq. (93), and the coefficients of the left side may be rewritten using the differential equation (60) and the Wronskian relation (75) as

$$\frac{d}{dz}\left\{\frac{\dfrac{d}{dz}\left[\left(\dfrac{\pi z}{2}\right)^{\frac{1}{2}} J_\nu(z)\right]}{\dfrac{d}{dz}\left[\left(\dfrac{\pi z}{2}\right)^{\frac{1}{2}} Y_\nu(z)\right]}\right\}_{z=\bar{j}_{\nu,s}'} = \left(\frac{4\nu^2-1}{4(\bar{j}'_{\nu,s})^2} - 1\right)\left[\left(\frac{\pi}{2}\bar{j}'_{\nu,s}\right)^{\frac{1}{2}} J_\nu(\bar{j}'_{\nu,s})\right]^2. \tag{94}$$

The first approximation for ϵ is then

$$\epsilon \sim \frac{\pi}{2K \ln(K/\bar{j}'_{0,s})[(4(\bar{j}'_{0,s}))^{-2}+1][(\frac{1}{2}\pi\bar{j}'_{0,s})^{\frac{1}{2}} J_0(\bar{j}'_{0,s})]^2}, \qquad \nu = 0,$$

$$\sim \frac{\pi(\nu+\frac{1}{2})(\bar{j}'_{\nu,s}/2K)^{2\nu}}{K\left(\dfrac{4\nu^2-1}{4(\bar{j}'_{\nu,s})^2}-1\right)\left[\left(\dfrac{\pi\bar{j}'_{\nu,s}}{2}\right)^{\frac{1}{2}} J_\nu(\bar{j}'_{\nu,s})\right]^2 (\nu-\frac{1}{2})\Gamma(\nu)\Gamma(\nu+1)}, \qquad \nu > 0, \quad \nu \neq \tfrac{1}{2}, \tag{95}$$

which is $o(K)$, so that $\epsilon \to 0$ faster than $1/K$ as $K \to \infty$. Thus, indeed, in this limit, $\bar{x}'_{\nu,K,s} \sim \bar{j}'_{\nu,s}/K$. Again, in the case $\nu = l + \frac{1}{2}$, l integral, we may use the power-series expansions of (76), (77), and so obtain an expression for ϵ in descending powers of K. For $l > 0$,

$$\epsilon \sim \frac{(\bar{j}'_{l+\frac{1}{2},s})^{2l+1}}{K^{2l+2}\left[\dfrac{l(l+1)}{(\bar{j}'_{l+\frac{1}{2},s})^2}-1\right](j_l(\bar{j}'_{l+\frac{1}{2},s}))^2}\,\frac{(l+1)(2l+1)}{l[1\cdot 3\cdot 5\cdots(2l+1)]^2} + O(K^{-2l-4}). \tag{96}$$

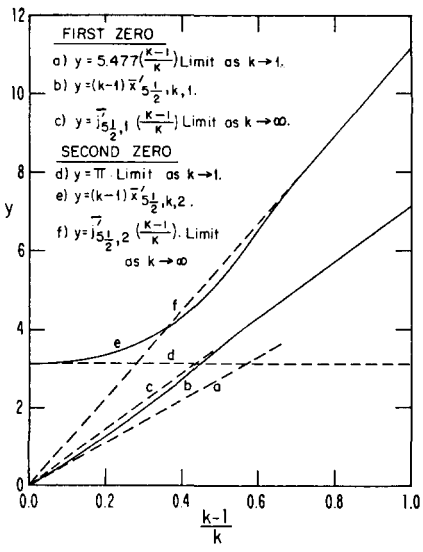


FIG. 11. First two zeros of

$$\frac{d(xj_5(x))/dx}{d(xy_5(x))/dx} - \frac{d(xj_5(Kx))/dx}{d(xy_5(Kx))/dx}$$

as a function of K. The dependence on the parameter K of the zeros $\bar{x}'_{5\frac{1}{2},K,s}$ of (86) for $\nu = 5\frac{1}{2}$ is illustrated by the solid curves b and e. The broken curves indicate the limiting behavior as $K \to 1$ and $K \to \infty$. The values of the zeros $\bar{j}'_{5\frac{1}{2},s}$ of $d(xj_5(x))/dx$ are $\bar{j}'_{5\frac{1}{2},1} = 7.140227364003$, $\bar{j}'_{5\frac{1}{2},2} = 11.18898477565$.

The value 5.477 in curve a is the first maximum of

$$\frac{d(xj_5(x))/dx}{d(xy_5(x))/dx},$$

which is plotted in Fig. 9.

When ν is large, we may apply the asymptotic expansions for $\bar{j}'_{\nu,s}$ and $(\frac{1}{2}\pi\bar{j}'_{\nu,s})^{\frac{1}{2}}J_\nu(\bar{j}'_{\nu,s})$ obtained in Sec. 1.

In the considerations above, the case $\nu = \frac{1}{2}$, $l = 0$, is excluded as anomalous. This arises because

$$\frac{d(xj_0(x))/dx}{d(xy_0(x))/dx} = \cot(x) \tag{97}$$

becomes infinite rather than zero as $x \to 0$. However, the zeros for this case are readily handled. The zeros of (87), $l = 0$, satisfy

$$\cot(x) = \cot(Kx), \tag{98}$$

so that

$$\bar{x}'_{\frac{1}{2},K,s} = \pi(s-1)/(K-1), \quad s = 1, 2, \cdots. \tag{99}$$

The behavior of the first two zeros $\bar{x}'_{\nu,K,s}$ for $\nu = 5\frac{1}{2}$ is illustrated in Fig. 11. Because the normalization was chosen for illustrating the $K \to 1$ limit conveniently, the limit $K \to \infty$ of interest here is represented by the approach to the straight lines through the origin.

Limit as $\nu \to \infty$

Inasmuch as the functions $J_\nu(x)/Y_\nu(x)$ and

$$\frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x)\right]}$$

both have for large ν an increasingly slow rise from the small values at small x, we may repeat the argument made for the zeros $x_{\nu,K,s}$ of (64) to realize that here, in complete analogy, as $\nu \to \infty$, $\bar{x}'_{\nu,K,s} \to \bar{j}'_{\nu,s}/K$ for any fixed $K > 1$. The procedure is just as before, using the Debye asymptotic expansions. If $\bar{x}'_{\nu,K,s} = (\bar{j}'_{\nu,s}/K) + \epsilon$, then

$$\epsilon\frac{d}{dx}\left(\frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(Kx)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(Kx)\right]}\right)_{x=\bar{j}_{\nu,s}'/K} + \frac{\epsilon^2}{2!}\frac{d^2}{dx^2}\left(\frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(Kx)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(Kx)\right]}\right)_{x=\bar{j}_{\nu,s}'/K} + \cdots$$

$$= \left(\frac{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}J_\nu(x)\right]}{\dfrac{d}{dx}\left[\left(\dfrac{\pi x}{2}\right)^{\frac{1}{2}}Y_\nu(x)\right]}\right)_{x=(\bar{j}_{\nu,s}'/K)+\epsilon}$$

$$= \left(\frac{J'_\nu(x) + \dfrac{1}{2x}J_\nu(x)}{Y'_\nu(x) + \dfrac{1}{2x}Y_\nu(x)}\right)_{x=(\bar{j}_{\nu,s}'/K)+\epsilon}, \tag{100}$$

where $J_\nu((\bar{j}'_{\nu,s}/K) + \epsilon)$, $Y_\nu((\bar{j}'_{\nu,s}/K) + \epsilon)$ are taken from the Debye expansions (80), (81), and

$$J'_\nu\left(\frac{\bar{j}'_{\nu,s}}{K} + \epsilon\right) \sim \left(\frac{\sinh 2\beta'}{4\pi\nu}\right)^{\frac{1}{2}} \times \exp[\nu(\tanh\beta' - \beta')]\left[1 + \sum_{r=1}^{\infty}\frac{v_r(\coth\beta')}{\nu^r}\right], \tag{101}$$

$$Y'_\nu\left(\frac{\bar{j}'_{\nu,s}}{K} + \epsilon\right) \sim \left(\frac{\sinh 2\beta'}{\pi\nu}\right)^{\frac{1}{2}} \times \exp[-\nu(\tanh\beta' - \beta')]\left[1 + \sum_{r=1}^{\infty}\frac{(-1)^r v_r(\coth\beta')}{\nu^r}\right], \tag{102}$$

where

$$\operatorname{sech}\beta' = \frac{\bar{j}'_{\nu,s}}{\nu K} + \frac{\epsilon}{\nu} \tag{103}$$

with $v_r(t)$ polynomials

$$v_1(t) = \tfrac{1}{24}(-9t + 7t^3),$$

$$v_2(t) = \tfrac{1}{1152}(-135t^2 + 594t^4 - 455t^6), \cdots. \tag{104}$$

Now since $\bar{j}'_{\nu,s} \sim \nu + \alpha_1\nu^{\frac{1}{3}} + \alpha_2\nu^{-\frac{1}{3}} + \cdots$, we see that for all ν greater than some ν_0 depending on $K > 1$, we can find a $\beta'_\nu > 0$ such that $\operatorname{sech}\beta'_\nu = \bar{j}'_{\nu,s}/K$. Then

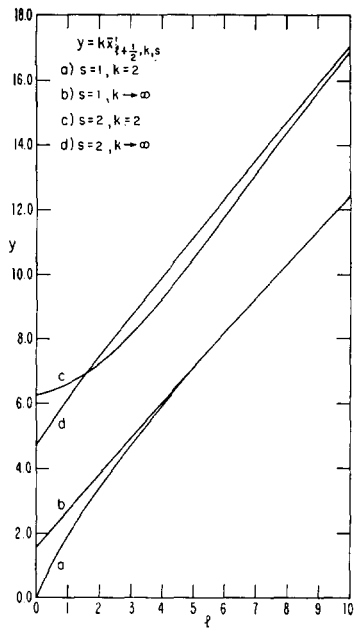


FIG. 12. First two zeros of

$$\frac{d(xj_l(x))/dx}{d(xy_l(x))/dx} - \frac{d(xj_l(Kx))/dx}{d(xy_l(Kx))/dx}$$

for $0 \leq l \leq 10$, $K = 2$, $K \to \infty$. The first two zeros $\bar{x}'_{l+\frac{1}{2},K,s}$ of (86) for $0 \leq l \leq 10$ are given as $K\bar{x}'_{l+\frac{1}{2},K,s}$ for $K = 2$, $K \to \infty$. As l increases, the values for any finite K approach the values $\bar{j}'_{l+\frac{1}{2},s}$ of the $K \to \infty$ limit.

the first approximation to ϵ is

$$\epsilon \sim \frac{\exp[2\nu(\tanh\beta'_\nu - \beta'_\nu)]}{4K\left(\frac{4\nu^2-1}{4(\bar{j}'_{\nu,s})^2} - 1\right)\left[\left(\frac{\pi\bar{j}'_{\nu,s}}{2}\right)^{\frac{1}{2}} J_\nu(\bar{j}'_{\nu,s})\right]^2}, \quad (105)$$

where the denominator has been written using (94). As was found in Eq. (85), so here ϵ becomes exponentially small as $\nu \to \infty$. The asymptotic expansions (49) and (58) from Sec. 1 should be introduced for $\bar{j}'_{\nu,s}$ and $J_\nu(\bar{j}'_{\nu,s})$.

Figure 12, showing $K\bar{x}'_{\nu,K,s}$ for $\frac{1}{2} \leq \nu \leq 10\frac{1}{2}$, illustrates the approach of the zeros $\bar{x}'_{\nu,K,s}$ of (86) to the zeros $\bar{j}'_{\nu,s}/K$ of $d[(\frac{1}{2}\pi x)^{\frac{1}{2}}J_\nu(Kx)]/dx$ as ν increases.

Numerical Computations for Figures

The calculations for the data presented in the figures were made with FORTRAN IV double-precision arithmetic on the IBM 7094 computer. All of the graphs present data for half-odd integral orders ν (integral orders l). The values for the functions were found using the relationships to the trigonometric functions

$$j_0(x) = (\sin x)/x, \quad y_0(x) = -(\cos x)/x,$$
$$j_1(x) = (\sin x)/x^2 - (\cos x)/x,$$
$$y_1(x) = -(\cos x)/x^2 - (\sin x)/x, \quad (106)$$

and recurrence relations for the spherical Bessel functions $f_l(x) = j_l(x), y_l(x)$,

$$\frac{2l+1}{x} f_l(x) = f_{l-1}(x) + f_{l+1}(x). \quad (107)$$

Zeros were obtained by using Newton's rule, that if z_1 is an approximation to a zero of $f(x)$, then $z_1 - f(z_1)/f'(z_1)$ is a closer approximation. The derivative $f'_l(x)$ required was found from the recurrence formula

$$(2l+1)f'_l(x) = lf_{l-1}(x) - (l+1)f_{l+1}(x). \quad (108)$$

ACKNOWLEDGMENT

I would like to thank Professor S. L. Glashow for making available to me the funds used in this research.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Conserved Quantities of Newman and Penrose*

DAVID C. ROBINSON†
Syracuse University, Syracuse, New York

(Received 26 February 1969)

Green's theorem is used to obtain the Newman–Penrose constants in flat and asymptotically flat space–time and to investigate the invariant transformations which these quantities generate. The zero-rest-mass free fields and the coupled Einstein–Maxwell fields are considered and the relationship of this approach to Noether's theorems is discussed.

1. INTRODUCTION

Recent investigations have shown that for a certain class of field theories, which includes zero-rest-mass fields and general relativity, weak conservation laws can be obtained by the use of Green's theorem.[1] Goldberg has used this result to calculate the Newman–Penrose (N.P.) constants for the massless scalar and Maxwell fields in Minkowski space and to identify the invariant transformations generated by these quantities.[2] It is the purpose of this paper to extend these considerations to asymptotically flat space–time and to indicate how the Green's theorem approach is related to the usual Noether theorem derivation of conservation laws.

First the Green's theorem method of obtaining weak conservation laws in curved and flat space–times is reviewed, and the connection with the Noether equation for the zero-rest-mass fields of spin one and two is exhibited. The leading N.P. constants for the zero-rest-mass fields in Minkowski space–time are then calculated using this technique, and the invariant transformations which these quantities generate are found. Next the N.P. constants for asymptotically flat space–time are considered within the context of the conformal approach of Penrose.[3] In this case the Green's identity is employed in the compactified manifold, conformal to physical space–time, and leads to constants which may be identified with the N.P. constants. Finally, the case of the coupled Einstein–Maxwell fields is considered, and it is found that when the Green's theorem expression is modified by the addition of the appropriate source term the N.P. constants for these fields are achieved.

* Work supported in part by the National Science Foundation; based on the author's doctoral dissertation at Syracuse University.

† National Academy of Sciences Postdoctoral Resident Research Associate. Present address: Aerospace Research Laboratories, Wright-Patterson Air Force Base, Ohio.

[1] J. N. Goldberg and E. T. Newman, J. Math. Phys. **10**, 369 (1969).

[2] E. T. Newman and R. Penrose, Phys. Rev. Letters **15**, 231 (1965); J. N. Goldberg, J. Math. Phys. **8**, 2161 (1967); **9**, 674 (1968).

[3] R. Penrose, Phys. Rev. Letters **10**, 66 (1963); R. Penrose, "Conformal Treatment of Infinity," in *Relativity Groups and Topology: the 1963 Les Houches Lectures*, C. DeWitt and B. DeWitt, Eds. (Gordon and Breach, Science Publishers, New York, 1964).

2. CONVENTIONS AND FORMALISMS

In general the conventions followed will be those of Ref. 4. The metric tensor $g_{\mu\nu}$ has signature $+ - - -$; covariant differentiation is denoted by "∇" and ordinary differentiation by "∂" and "," subscript; round and square brackets indicate symmetrization and antisymmetrization of indices in the usual manner.

The Riemann, Ricci, and conform tensors are defined by

$$\nabla_{[\sigma}\nabla_{\rho]}k_\nu = \tfrac{1}{2}R^{\mu}{}_{\nu\rho\sigma}k_\mu, \tag{2.1}$$

$$R_{\nu\rho} = R^{\mu}{}_{\nu\rho\mu}, \tag{2.2}$$

$$C_{\mu\nu\rho\sigma} = R_{\mu\nu\rho\sigma} + \tfrac{1}{2}(g_{\mu\rho}R_{\nu\sigma} - g_{\mu\sigma}R_{\nu\rho} + g_{\nu\sigma}R_{\mu\rho} - g_{\nu\rho}R_{\mu\sigma}) + \tfrac{1}{6}R(g_{\mu\sigma}g_{\nu\rho} - g_{\mu\rho}g_{\nu\sigma}), \tag{2.3}$$

where Greek indices range from 0 to 3. Two-component spinors will be used in discussing the zero-rest-mass fields; since the development of this formalism by Penrose will be followed, only a brief summary is given here.[4,5] The Hermitian spin tensor $\sigma_\mu^{A\dot{X}}$, which is used to relate tensors and spinors, satisfies the equation

$$g_{\mu\nu}\sigma^{\mu}_{A\dot{X}}\sigma^{\nu}_{B\dot{Y}} = \epsilon_{AB}\epsilon_{\dot{X}\dot{Y}}, \tag{2.4}$$

where

$$\epsilon_{AB} = \epsilon_{\dot{A}\dot{B}} = \epsilon^{AB} = \epsilon^{\dot{A}\dot{B}}$$

and

$$\epsilon_{00} = \epsilon_{11} = 0, \quad \epsilon_{01} = -\epsilon_{10} = 1.$$

Latin capitals are used for spinor indices and take the values 0, 1; dotted and undotted indices refer to complex-conjugate spin spaces. The ϵ's act as raising and lowering operators for the spinor indices, the conventions being $o^A = \epsilon^{AB}o_B$, $o^B = o^A\epsilon_{AB}$ and similarly for dotted indices. Covariant differentiation for spinors is uniquely determined by the relations

$$\nabla_{A\dot{X}}\epsilon_{MN} = \nabla_{A\dot{X}}\sigma^{\mu}_{B\dot{Y}} = 0, \tag{2.5}$$

where

$$\nabla_{A\dot{X}} \equiv \sigma^{\mu}_{A\dot{X}}\nabla_\mu.$$

[4] E. T. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).

[5] R. Penrose, Ann. Phys (N.Y.) **10**, 171 (1960); R. Penrose and W. Rindler, Spinor Notes (unpublished).

Some useful correspondences between tensors and spinors are given by

$$C^{\mu\nu\rho\sigma} = -\sigma^{\mu}_{A\dot{W}}\sigma^{\nu}_{B\dot{X}}\sigma^{\rho}_{C\dot{Y}}\sigma^{\sigma}_{D\dot{Z}} \times [\Psi^{ABCD}\epsilon^{\dot{W}\dot{X}}\epsilon^{\dot{Y}\dot{Z}} + \bar{\Psi}^{\dot{W}\dot{X}\dot{Y}\dot{Z}}\epsilon^{AB}\epsilon^{CD}], \quad (2.6)$$

$$R^{\mu\nu} - \tfrac{1}{2}g^{\mu\nu}R = -\sigma^{\mu}_{A\dot{X}}\sigma^{\nu}_{B\dot{Y}}\Phi^{AB\dot{X}\dot{Y}}, \quad (2.7)$$

$$R^{\mu\nu} - \tfrac{1}{2}g^{\mu\nu}R = \sigma^{\mu}_{A\dot{X}}\sigma^{\nu}_{B\dot{Y}}G^{AB\dot{X}\dot{Y}}, \quad (2.8)$$

$$F^{\mu\nu} = \sigma^{\mu}_{A\dot{X}}\sigma^{\nu}_{B\dot{Y}}[\Phi^{AB}\epsilon^{\dot{X}\dot{Y}} + \bar{\Phi}^{\dot{X}\dot{Y}}\epsilon^{AB}], \quad (2.9)$$

where $F^{\mu\nu}$ is the Maxwell field tensor and $G_{AB\dot{X}\dot{Y}}$ the Einstein spinor and

$$\Phi_{AB} = \Phi_{(AB)}, \quad \Psi_{ABCD} = \Psi_{(ABCD)},$$
$$\Phi_{AB\dot{X}\dot{Y}} = \Phi_{(AB)(\dot{X}\dot{Y})} = \bar{\Phi}_{\dot{X}\dot{Y}AB}.$$

Using these results, the Ricci identities may be written in terms of spinors as

$$\nabla_{(A}{}^{\dot{P}}\nabla_{B)\dot{P}}\xi_C \equiv -\Psi_{ABCD}\xi^D + \tfrac{1}{12}R\xi_{(A}\epsilon_{B)C},$$
$$\nabla_{C(\dot{P}}\nabla^{C}{}_{\dot{Q})}\xi_A \equiv \Phi_{AB\dot{P}\dot{Q}}\xi^B \quad (2.10)$$

and the Bianchi identities become

$$\nabla^{D}{}_{\dot{G}}\Psi_{ABCD} \equiv \nabla_{(C}{}^{\dot{H}}\Phi_{AB)\dot{G}\dot{H}},$$
$$\nabla^{A\dot{G}}\Phi_{AB\dot{G}\dot{H}} \equiv -\tfrac{1}{8}\nabla_{B\dot{H}}R. \quad (2.11)$$

3. GREEN'S THEOREM AND THE NOETHER EQUATION

The zero-rest-mass free field equations for spin s, $s > 0$, integral or half integral, are

$$\nabla^{A\dot{X}}\Phi_{AB\cdots K} = 0, \quad (3.1)$$

where $\Phi_{AB\cdots K}$ is a totally symmetric spinor with $2s$ indices.[6] Differentiating (3.1) and using the Ricci identities gives

$$\nabla_{A\dot{X}}\nabla^{Y\dot{X}}\Phi_{YB\cdots K} \equiv \boxtimes\Phi_{AB\cdots K} = 0. \quad (3.2)$$

The operator $\boxtimes$ is defined by

$$\boxtimes\Phi_{AB\cdots K} \equiv \tfrac{1}{2}\Box\Phi_{AB\cdots K} + \frac{R}{24}(2s+2)\Phi_{AB\cdots K} + \tfrac{1}{2}(\Psi_A{}^Y{}_{BX}\Phi_Y{}^X{}_{C\cdots K} + \Psi_A{}^Y{}_{CX}\Phi_{YB}{}^X{}_{\cdots K} + \cdots + \Psi_A{}^Y{}_{KX}\Phi_{YBC\cdots}{}^X) \quad (3.3)$$

and reduces to the D'Alembertian $\Box$ in flat space-time.

If $H^{AB\cdots K}$ is a totally symmetric spinor, then a Green's identity may be written

$$H^{AB\cdots K}\boxtimes\Phi_{AB\cdots K} - \Phi_{AB\cdots K}\boxtimes H^{AB\cdots K} \equiv \tfrac{1}{2}\nabla^{X\dot{Y}}(H^{AB\cdots K}\nabla_{X\dot{Y}}\Phi_{AB\cdots K} - \Phi_{AB\cdots K}\nabla_{X\dot{Y}}H^{AB\cdots K}). \quad (3.4)$$

Consequently, if $H^{AB\cdots K}$ satisfies the equation

$$\boxtimes H^{AB\cdots K} = 0, \quad (3.5)$$

a weak conservation law is obtained when the field equations (3.1) are satisfied. This is given by

$$\nabla^{X\dot{Y}}t_{(s)X\dot{Y}} = 0, \quad (3.6)$$

where

$$t_{(s)X\dot{Y}} \equiv H^{AB\cdots K}\nabla_{X\dot{Y}}\Phi_{AB\cdots K} - \Phi_{AB\cdots K}\nabla_{X\dot{Y}}H^{AB\cdots K}. \quad (3.7)$$

A similar result holds of course for the case $s = 0$, which is trivial, and will not be considered here.

Now for fields with equations derivable from a variational principle, Noether's theorems apply and lead to the Noether equation

$$-\delta y_A L^A = t^{A\dot{X}}{}_{,A\dot{X}}, \quad (3.8)$$

where δy_A is the invariant transformation and $L^A = 0$ are the field equations in the field variables y_A.[7] When the field equations are satisfied, (3.8) leads to the weak conservation law $t^{A\dot{X}}{}_{,A\dot{X}} = 0$; when $t^{A\dot{X}}$ depends locally on the field variables, construction of this equation enables the invariant transformation δy_A, generated by the conserved quantity, to be identified.

For $s = 0, \frac{1}{2}, 1, 2$, it is a simple matter to relate the above use of Green's theorem to the appropriate Noether equations. For example, for $s = 1$, we have the identity in the field variables

$$\nabla_{D\dot{X}}H^{DB}\nabla^{A\dot{X}}\Phi_{AB} = \nabla_{D\dot{X}}[H^{DB}\nabla^{A\dot{X}}\Phi_{AB} - \tfrac{1}{2}t_{(1)}{}^{D\dot{X}}] \quad (3.9)$$

and, for $s = 2$,

$$\nabla_{D\dot{Y}}\nabla_{A\dot{X}}H^{ABCD}G_{BC}{}^{\dot{X}\dot{Y}} = \nabla_{D\dot{X}}[\nabla_{A\dot{Y}}H^{ABCD}G_{BC}{}^{\dot{X}\dot{Y}} - H^{ABCD}\nabla_{A\dot{Y}}G_{BC}{}^{\dot{X}\dot{Y}} + \tfrac{1}{2}t_{(2)}{}^{D\dot{X}}], \quad (3.10)$$

where H^{DB} and H^{ABCD} satisfy Eq. (3.5). These equations have the form of Noether's equations, give rise to the same conserved quantities as Green's theorem, and may be used to identify the invariant transformations which these quantities generate. In flat space-time, the $H^{AB\cdots K}$ are the generalized Hertz

[6] When the vacuum Einstein equations are satisfied, Φ_{ABCD} is identified with the conform spinor Ψ_{ABCD}.

[7] A. Trautman, "Conservation Laws," in *Gravitation*, L. Witten, Ed. (John Wiley & Sons, New York, 1962).

potentials for spin-s fields.[8] In curved space–time this is true only for the Maxwell field.

4. THE N.P. CONSTANTS IN FLAT SPACE-TIME

In flat space-time, $\Psi_{ABCD} = R = 0$ and Eq. (3.5) reduces to

$$\Box H^{AB\cdots K} = 0. \tag{4.1}$$

The fundamental two-point solution of this equation is

$$H^{AB\cdots K}_{A'B'\cdots K'} \equiv \delta^{AB\cdots K}_{A'B'\cdots K'} D(x - x'), \tag{4.2}$$

where $D(x - x')$ is the free-field propagator

$$D(x - x') = (4\pi p)^{-1}[\delta(v_\mu(x^\mu - x^{\mu'}) - p) - \delta(v_\mu(x^\mu - x^{\mu'}) + p)] \tag{4.3}$$

and

$$\epsilon_{\mu\sigma} = v_\mu v_\sigma - g_{\mu\sigma}, \quad p = [\epsilon_{\mu\sigma}(x^\mu - x^{\mu'})(x^\sigma - x^{\sigma'})]^{\frac{1}{2}}, \quad v^\mu v_\mu = 1.$$

The symmetric spinor $\delta^{AB\cdots K}_{A'B'\cdots K'}$ is a parallel propagator in flat space, a constant spinor as a function of x (unprimed indices) and x' (primed indices). In order to investigate the conserved quantity which this choice of $H^{AB\cdots K}$ gives rise to, we integrate (3.6) over the region R_4 in Fig. 1.

By the use of Gauss's theorem we obtain

$$\Phi_{A'B'\cdots K'}(x') = 2\int_N \delta^{AB\cdots K}_{A'B'\cdots K'}[\Phi_{AB\cdots K}\nabla^{X\dot{Y}} D(x-x') - \nabla^{X\dot{Y}}\Phi_{AB\cdots K} D(x - x')]\, dS_{X\dot{Y}}. \tag{4.4}$$

In order to reduce the integrand to independent data on N, it is convenient to use the spinor dyad formalism of Newman and Penrose.[4] A spinor dyad (o_A, ι_A) is introduced at each point of space–time, with the normalization

$$o_A\iota^A = 1. \tag{4.5}$$

When the dyad components of the field

$$\Phi_n = \Phi_{AB\cdots PQ\cdots K} o^A o^B \cdots o^P \iota^Q \cdots \iota^K \tag{4.6}$$

(n is the number of ι_A's and ranges from 0 to $2s$) and the intrinsic derivatives

$$D \equiv o^A\bar{o}^{\dot{X}}\nabla_{A\dot{X}}, \quad \Delta \equiv \iota^A\bar{\iota}^{\dot{X}}\nabla_{A\dot{X}}, \quad \delta \equiv o^A\bar{\iota}^{\dot{X}}\nabla_{A\dot{X}} \tag{4.7}$$

are introduced, the field equations (3.1) may be written[9]

$$\begin{aligned}\Delta\Phi_{n-1} - \delta\Phi_n - (n-1)\nu\Phi_{n-2} &+ (n\mu + 2(n-s-1)\gamma)\Phi_{n-1} \\ &+ (2(s-n)\beta + (2s-n+1)\tau)\Phi_n \\ &+ (n-2s)\sigma\Phi_{n+1} = 0,\end{aligned} \tag{4.8a}$$

$$\begin{aligned}D\Phi_n - \bar{\delta}\Phi_{n-1} + (n-1)\lambda\Phi_{n-2} &+ (2(s-n+1)\alpha - n\pi)\Phi_{n-1} \\ &+ (2(n-s)\epsilon + (n-2s-1)\rho)\Phi_n \\ &+ (2s-n)\kappa\Phi_{n+1} = 0, \quad n = 1, \cdots, 2s.\end{aligned} \tag{4.8b}$$

The spin coefficients are given by

$$\begin{aligned}\kappa &= o^A Do_A, & \epsilon &= \iota^A Do_A, & \pi &= \iota^A D\iota_A, \\ \rho &= o^A\bar{\delta}o_A, & \alpha &= \iota^A\bar{\delta}o_A, & \lambda &= \iota^A\bar{\delta}\iota_A, \\ \sigma &= o^A\delta o_A, & \beta &= \iota^A\delta o_A, & \mu &= \iota^A\delta\iota_A, \\ \tau &= o^A\Delta o_A, & \gamma &= \iota^A\Delta o_A, & \nu &= \iota^A\Delta\iota_A.\end{aligned} \tag{4.9}$$

If the dyad is chosen so that

$$o_A\bar{o}_{\dot{X}} = u_{,A\dot{X}}$$

and

$$\iota_A\bar{\iota}_{\dot{X}} = v_{,A\dot{X}},$$

where v = constant denotes the retrograde null cone from x', the phases of the dyad spinors may be adjusted so that the only nonzero spin coefficients are[10]

$$\rho = 2\mu, \quad \alpha = -\beta. \tag{4.10}$$

Then Eq. (4.4) reduces to

$$\Phi_{A'B'\cdots K'}(x') = 2\int_N \delta^{AB\cdots K}_{A'B'\cdots K'} D(x-x')[D\Phi_{AB\cdots K} - \rho\Phi_{AB\cdots K}]dV. \tag{4.11}$$

Now,

$$\Phi_{AB\cdots K} = (-1)^{2s}\left[\Phi_0\iota_A\cdots\iota_K + \sum_{n=0}^{2s-1}\Phi_{n+1}\frac{2s!\,(-1)^{n+1}}{(n+1)!\,(2s-n-1)!}\iota_{(A}\cdots\iota_P o_Q\cdots o_{K)}\right], \tag{4.12}$$

where the indices $A\cdots P$ number $(2s - n - 1)$. By using (4.8), (4.10), and (4.12), the integrand of (4.11)

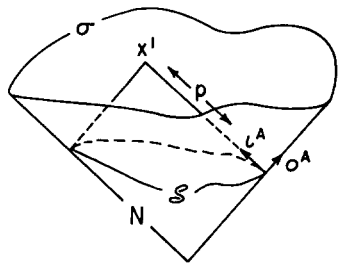


FIG. 1. The region R_4 is bounded by an outgoing null cone N given by u = const, and a spacelike hypersurface, σ, containing the point x'.

[8] R. Penrose, Proc. Roy. Soc. (London) **A284**, 159 (1965). This identification of the Hertz potentials was made by Goldberg and Newman.

[9] E. Grgin, Ph.D. dissertation, Syracuse University, 1966.

[10] A. Janis and E. T. Newman, J. Math. Phys. **6**, 902 (1965).

may be reduced to

$$(-1)^{2s}D(x-x')\delta^{AB\cdots K}_{A'B'\cdots K'}\iota_A\iota_B\cdots\iota_K[D\Phi_0-\rho\Phi_0]$$
$$+(-1)^{2s}D(x-x')\delta^{AB\cdots K}_{A'B'\cdots K'}$$
$$\times\sum_{n=0}^{2s-1}(-1)^{n+1}\frac{2s!}{(n+1)!\,(2s-n-1)!}$$
$$\times\rho[(n+1)\Phi_n\iota_A\cdots\iota_P\iota_Q o_R\cdots o_K$$
$$+(2s-n-1)\Phi_{n+1}\iota_A\cdots\iota_P o_Q o_R\cdots o_K]$$
$$+D(x-x')\sum_{n=0}^{2s-1}(-1)^{2s+n+1}$$
$$\times\frac{2s!}{(n+1)!\,(2s-n-1)!}A_{n+1}, \quad (4.13)$$

where

$$A_{n+1}\equiv(\bar\delta-2\alpha)(\Phi_{n+1}\iota_A\cdots\iota_P o_Q\cdots o_K\delta^{A\cdots PQ\cdots K}_{A'\cdots P'Q'\cdots K'}). \quad (4.14)$$

The terms A_{n+1} make no contribution to the integral. In order to see this, it is convenient to introduce an affine parameter r along the null geodesics in the outgoing null cones $u=$ const. Then when this parameter is adjusted so that

$$o^A\bar o^{\dot X}\nabla_{A\dot X}r=1 \quad (4.15)$$

and $r=r'$ at $\mathcal{S}$, the terms in the integral involving A_{n+1} become proportional to the integral over the sphere

$$\int\bar\delta\chi\,dS,$$

where χ has spin weight one. Consequently, these terms are zero.[11]

Hence (4.11) reduces to

$$\Phi_{A'B'\cdots K'}=\frac{(-1)^{2s}}{2\pi}\int_{\mathcal{S}}\frac{1}{p}\delta^{A\cdots K}_{A'\cdots K'}\iota_A\cdots\iota_K$$
$$\times[D-(2s+1)\rho]\Phi_0\,dS, \quad (4.16)$$

where

$$\rho=-r^{-1}.$$

If a different scaling of the dyad spinors [consistent with (4.5)] is chosen, the expression takes the form

$$\Phi_{A'B'\cdots K'}=\frac{(-1)^{2s}}{2\pi}\int_{\mathcal{S}}\frac{1}{p}\delta^{A\cdots K}_{A'\cdots K'}\iota_A\cdots\iota_K\mathfrak{D}\Phi_0\,dS, \quad (4.17)$$

where

$$\mathfrak{D}\Phi_0\equiv[D-(2s+1)\rho-2s\epsilon]\Phi_0. \quad (4.18)$$

This is the standard form of the Kirchhoff integral, a result first obtained by Penrose.[12]

When the field peels[13] so that Φ_0 may be expanded in inverse powers of r,

$$\Phi_0=\sum_{n=0}^{N-(2s+1)}\Phi_0^n r^{-(2s+1+n)}+O(r^{-N}), \quad (4.19)$$

it follows that

$$r^{2s+3}\mathfrak{D}\Phi_0=-\Phi_0^1+O(r^{-1}). \quad (4.20)$$

Hence the weighted value of the field at timelike infinity is equal to an integral over the sphere at null infinity $\mathcal{S}_\infty$:

$$\lim_{p(x')\to\infty}[p(x')]^{2s+2}\Phi_{A'\cdots K'}(x')$$
$$=\frac{(-1)^{2s+1}}{2\pi}\int_{\mathcal{S}_\infty}\iota_{A'}\cdots\iota_{K'}\Phi_0^1\,dS. \quad (4.21)$$

Since the value of this integral is independent of the particular limiting two-surface $\mathcal{S}_\infty$ over which it is calculated, it is a constant of the motion. As Goldberg and Penrose have pointed out,[2,14] the spinors $\iota^{A'}\cdots\iota^{K'}$ give a representation of the spin-weighted spherical harmonics ${}_s\bar Y_{sm}$ and the constants given by (4.21) are the N.P. constants

$$C_{s,m}=\int{}_s\bar Y_{sm}\Phi_0^1\,dS. \quad (4.22)$$

It follows from (4.2) and the results of the previous section that the invariant transformations generated by these quantities are zero at all finite points of space–time.

5. CONFORMAL SPACE

The structure of curved space–time lacks sufficient symmetry to allow the propagator approach of flat space–time to be employed at finite distances from the sources. In curved space–time the propagators are not, in general, well defined and the field cannot be clearly separated into advanced and retarded components. However, the constants are defined at null infinity and it has been seen that in flat space–time the invariant transformations which they generate are essentially delta functions with support on the retrograde null cone at infinity. These considerations suggest that the curved-space problem is best approached via the conformal technique of Penrose where attention is focused on null infinity itself.[3,8]

In this approach, the necessary analytical and topological conditions for a space–time $(\tilde M,\tilde g_{\mu\nu})$ to be

[11] E. T. Newman and R. Penrose, J. Math. Phys. 7, 863 (1966); J. N. Goldberg, A. J. MacFarlane, F. Rohrlich, E. C. G. Sudarshan, and E. T. Newman, J. Math. Phys. 8, 2155 (1967).

[12] R. Penrose, "Null Hypersurface Initial Data," in P. G. Bergmann's Aeronautical Research Lab. Tech. Documentary Rept. 63-56 (Office of Aerospace Research, U.S. Air Force, 1963).

[13] R. K. Sachs, Proc. Roy. Soc. (London) **A270**, 103 (1962).

[14] E. T. Newman and R. Penrose, Proc. Roy. Soc. (London) **A305**, 175 (1968).

asymptotically flat are formulated by requiring the existence of a manifold $(M, g_{\mu\nu})$ conformal to the physical manifold in which null infinity $\mathfrak{I}$ appears as a regular hypersurface. The metric

$$g_{\mu\nu} = \Omega^2 \tilde{g}_{\mu\nu}, \quad g^{\mu\nu} = \Omega^{-2}\tilde{g}^{\mu\nu} \tag{5.1}$$

and the conformal factor Ω are required to be regular at $\mathfrak{I}$, which consists of two disjoint surfaces, future null infinity $\mathfrak{I}^+$, and past null infinity $\mathfrak{I}^-$. These surfaces and given by $\Omega = 0$, $\nabla_\mu \Omega \neq 0$ and have topology $S^2 \times E^1$. In order to make the meaning of distributions and derivatives at $\mathfrak{I}$ clear, M is considered as an open region of some manifold N, such that $\mathfrak{I}$ is completely within N. Calculations are performed in $(M, g_{\mu\nu})$ and the conformally invariant results given a physical space interpretation.

The transformation formulas between quantities in $\tilde{M}$ and M have been developed and it will be convenient to list them here using the tilde notation of Penrose.

The basic transformation formulas are chosen to preserve Eq. (2.4):

$$\tilde{\sigma}_\mu^{A\dot{B}} = \Omega^{-1}\sigma_\mu^{A\dot{B}}, \quad \tilde{\sigma}^\mu_{A\dot{B}} = \Omega\sigma^\mu_{A\dot{B}},$$
$$\tilde{\epsilon}_{AB} = \epsilon_{AB}. \tag{5.2}$$

Then,

$$\tilde{\Psi}_{ABCD} = \Omega^2 \Psi_{ABCD}, \tag{5.3}$$

$$\tilde{\Phi}_{AB}^{\dot{C}\dot{D}} = \Omega^2 \Phi_{AB}^{\dot{C}\dot{D}} + \Omega\nabla_{(A}{}^{\dot{C}}\nabla_{B)}{}^{\dot{D}}\Omega, \tag{5.4}$$

$$\tilde{R} = \Omega^2 R - 6\Omega\nabla_{A\dot{B}}\nabla^{A\dot{B}}\Omega + 12\nabla_{A\dot{B}}\Omega\nabla^{A\dot{B}}\Omega. \tag{5.5}$$

The correspondences for the rest-mass-zero fields are chosen so that the free fields are conformally invariant. This gives, for spin s,

$$\tilde{\Phi}_{AB\cdots K} = \Omega^{s+1}\Phi_{AB\cdots K}, \tag{5.6a}$$

$$\tilde{\nabla}^{A\dot{X}}\tilde{\Phi}_{AB\cdots K} = \Omega^{s+2}\nabla^{A\dot{X}}\Phi_{AB\cdots K}, \tag{5.6b}$$

where for $s = 2$ we identify $\tilde{\Phi}_{ABCD}$ with the conform spinor $\tilde{\Psi}_{ABCD}$. For the Einstein–Maxwell field

$$\tilde{G}_{AB\dot{C}\dot{D}} = -\tilde{\Phi}_{AB}\tilde{\bar{\Phi}}_{\dot{C}\dot{D}}, \tag{5.7}$$

and the condition that Φ_{AB} be continuous at $\mathfrak{I}^+$ implies that

$$\Psi_{ABCD} = 0 \quad \text{at} \quad \mathfrak{I}^+ \tag{5.8}$$

and that the electromagnetic and gravitational fields peel. Similar results hold for the massless scalar and neutrino fields coupled to the gravitational field as well as for the uncoupled field. For such fields, (5.4) and (5.5) imply that, at $\mathfrak{I}^+$,

$$\nabla_{A\dot{B}}\Omega\nabla^{A\dot{B}}\Omega = 0, \tag{5.9}$$

$$\nabla_{(A}{}^{\dot{C}}\nabla_{B)}{}^{\dot{D}}\Omega = 0, \tag{5.10}$$

and consequently $\mathfrak{I}^+$ is null and shear free in these cases. In the following a particularly simple conformal space will be constructed and used in performing the calculations, the results of which will be shown to be conformally invariant.

Consider the space-time $(M^{(1)}, g^{(1)}_{\mu\nu})$, conformal to the asymptotically flat space-time $(\tilde{M}, \tilde{g}_{\mu\nu})$. The conformal factor Ω may be chosen to be an inverse luminosity parameter, in which case $\mathfrak{I}^+$ is shear free, divergence free, and has spacelike cross-sections which are unit spheres.[3]

Following Tamburino and Winicour, a "conformal Bondi frame" may be set up in this space.[15] An initial spacelike cross section of $\mathfrak{I}^+$, Σ, say, is chosen and assigned coordinates x^A $(A = 2, 3)$ so that

$$g^{(1)\alpha\beta}x^A_{,\alpha}x^B_{,\beta} = -\delta^{AB}P^2 \tag{5.11}$$

on Σ, where

$$\zeta = x^2 + ix^3, \quad P = \tfrac{1}{2}(1 + \zeta\bar{\zeta}). \tag{5.12}$$

An affine parameter u is assigned along the null geodesics in $\mathfrak{I}^+$, and the points on a given null geodesic are assigned the values x^A of its intersection with Σ. Then $x^0 = u$, x^A coordinatize $\mathfrak{I}^+$. These labels are extended into M by assigning the coordinate $x^0 = u$ to all points of the outgoing null hypersurface N which intersects $\mathfrak{I}^+$ in the spacelike cross section $u = \text{const}$, and x^A to all points in the null geodesic, lying in N, which intersects $\mathfrak{I}^+$ in the point $x^0 = u$, x^A.

Finally, $x^1 = R$ is defined by

$$R^4 = \Omega^4 \left| g^{\alpha\beta}x^A_{,\alpha}x^B_{,\beta} \right|. \tag{5.13}$$

By performing the conformal transformation $M^{(1)} \to M$ given by

$$g^{(1)}_{\mu\nu} = (R/\Omega)^{-2} g_{\mu\nu}, \tag{5.14}$$

a new unphysical space $(M, g_{\mu\nu})$ is achieved whose metric is related to the physical metric by

$$\tilde{g}_{\mu\nu} = R^{-2} g_{\mu\nu}. \tag{5.15}$$

At $\hat{\mathfrak{I}}^+$,

$$R = 0. \tag{5.16}$$

The coordinate and conformal conditions then give

$$|g_{AB}| = |g^{AB}| = 1,$$
$$g_{\mu\nu} = \begin{pmatrix} g_{00} & g_{01} & g_{0A} \\ g_{01} & 0 & 0 \\ g_{0A} & 0 & g_{AB} \end{pmatrix},$$
$$g^{\mu\nu} = \begin{pmatrix} 0 & g^{01} & 0 \\ g^{01} & g^{11} & g^{1A} \\ 0 & g^{1A} & g^{AB} \end{pmatrix}. \tag{5.17}$$

[15] L. Tamburino and J. Winicour, Phys. Rev. **150**, 1039 (1966).

Using (5.9) and (5.10), we have, at $\mathfrak{I}^+$,

$$g^{\mu\nu}R_{\mu\nu} = C_{\mu\nu\rho\sigma} = \Psi_{ABCD} = 0,$$
$$g_{00} = g_{00,1} = g_{0A} = g_{0A,1} = g_{01,1} = g_{AB,0} = 0,$$
$$g_{01} = 1, \quad (5.18)$$
$$g^{11} = g^{11}{}_{,1} = g^{1A} = g^{1A}{}_{,1} = g^{01}{}_{,1} = g^{AB}{}_{,0} = 0,$$
$$g^{01} = 1.$$

The fact that on the initial cross section on $\mathfrak{I}^+$, Σ,

$$g_{AB} = -\delta_{AB}$$

by construction, and that $g_{AB,0} = g^{AB}{}_{,0} = 0$ on $\mathfrak{I}^+$, gives at $\mathfrak{I}^+$

$$g^{AB} = -\delta^{AB}, \quad g_{AB} = -\delta_{AB}. \quad (5.19)$$

By writing the line element in M as

$$ds^2 = -(g_{01})^2 g^{11}\,du^2 + 2g_{01}\,du\,dR + g_{AB}(dx^A + U^A\,du)(dx^B + U^B\,du), \quad (5.20)$$

where

$$U^A = -g_{01}g^{1A},$$

it is easy to see that a suitable null tetrad in M is

$$l_\mu = u_{,\mu}, \quad n_\mu = -\tfrac{1}{2}(g_{01})^2 g^{11}u_{,\mu} + g_{01}R_{,\mu},$$
$$m_\mu = 2^{-\frac{1}{2}}(\tau_A x^A_{,\mu} + \tau_A U^A u_{,\mu}), \quad (5.21)$$

where

$$g_{AB} = -\tfrac{1}{2}(\tau_A\bar{\tau}_B + \bar{\tau}_A\tau_B) \quad (5.22)$$

and

$$g^{AB}\tau_A\tau_B = 0$$

define the dyad τ_A. At $\mathfrak{I}^+$ we have

$$\tau_A = \delta^2_A + i\delta^3_A, \quad (5.23a)$$
$$U^A = U^A_{,\nu} = 0. \quad (5.23b)$$

This null tetrad has the usual orthogonality and normalization properties

$$l_\mu n^\mu = -m_\mu\bar{m}^\mu = 1,$$
$$l_\mu l^\mu = n_\mu n^\mu = m_\mu m^\mu = m_\mu n^\mu = m_\mu l^\mu = 0, \quad (5.24)$$

and corresponds to the dyad (o^A, ι^A), where

$$o^A\bar{o}^{\dot{X}} = \sigma_\mu{}^{A\dot{X}}l^\mu,$$
$$\iota^A\bar{\iota}^{\dot{X}} = \sigma_\mu{}^{A\dot{X}}n^\mu, \quad (5.25)$$
$$\bar{o}^A\bar{\iota}^{\dot{X}} = \sigma_\mu{}^{A\dot{X}}m^\mu.$$

From (5.18), (5.19), (5.21), (5.23), and (5.25) it can easily be seen that at $\mathfrak{I}^+$ the only nonzero spin coefficients are σ and $\bar{\epsilon} - \epsilon$, and the latter may be eliminated by a dyad rotation. Since σ contains the radiation "news," it is clear that it cannot, in general, be eliminated at $\mathfrak{I}^+$. In the following, this dyad and conformal manifold will be referred to as "standard," for which, at $\mathfrak{I}^+$,

$$\nabla_{B\dot{X}}\iota^A = 0, \quad (5.26a)$$
$$\nabla_{B\dot{X}}o^A = \sigma\iota_B\bar{\iota}^A\bar{o}_{\dot{X}}. \quad (5.26b)$$

6. THE N.P. CONSTANTS IN ASYMPTOTICALLY FLAT SPACE-TIME FOR THE FREE FIELDS[14,16]

Using the coordinate and dyad results calculated above, it is a straightforward, if lengthy, matter to prove that a solution (in the usual sense of distributions) of the generalized wave equation (3.5) in M is given by

$$H^{AB\cdots K} = \mathfrak{W}o^A o^B \cdots o^K\delta(R), \quad (6.1)$$

where $\mathfrak{W}(\zeta)$ is an analytic function and $\delta(R)$ is a generalized delta function "concentrated on the surface $R = 0$."[17]

For the free fields,

$$\nabla^{A\dot{X}}\tilde{\Phi}_{ABCD} = 0. \quad (6.2)$$

When $\Phi^{AB\cdots K}$, given by (5.6a), is continuous at $\mathfrak{I}^+$, the Green's identity (3.4) in M leads to the weak conservation law

$$\nabla^{X\dot{Y}}(H_{AB\cdots K}\nabla_{X\dot{Y}}\Phi^{AB\cdots K} - \Phi^{AB\cdots K}\nabla_{X\dot{Y}}H_{AB\cdots K}) \equiv \nabla^{X\dot{Y}}t_{(s)X\dot{Y}} = 0. \quad (6.3)$$

Integrating this expression over the region R_4 in Fig. 2 and using Gauss's theorem and the fact that $\mathfrak{I}^+$ is the support of $H^{AB\cdots K}$ gives the conservation law:

$$\int_{\sigma_1}\mathfrak{W}D\Phi_0\,dS = \int_{\sigma_2}\mathfrak{W}D\Phi_0\,dS, \quad (6.4)$$

where

$$\sigma_i = N_i \cap \mathfrak{I}^+, \quad i = 1, 2.$$

Since $\rho = \epsilon = 0$ at $\mathfrak{I}^+$, the conserved quantities may be written using the operator "$\mathfrak{D}$," introduced in Sec. 3. Thus,

$$C_{s,m} \equiv \int_\sigma \mathfrak{W}\mathfrak{D}\Phi_0\,dS \quad (6.5)$$

are the conserved quantities.

Under the dyad transformation

$$o^{A'} = \chi^{-1}o^A, \quad \iota^{A'} = \chi\iota^A,$$
$$dS' = \chi\bar{\chi}\,dS, \quad (6.6)$$

and the spin coefficients transform according to the

[16] R. Penrose, "Conserved Quantities and Conformal Structure in General Relativity," in *Relativity Theory and Astrophysics*, J. Ehlers, Ed. (American Mathematical Society, Providence, R.I., 1967).

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

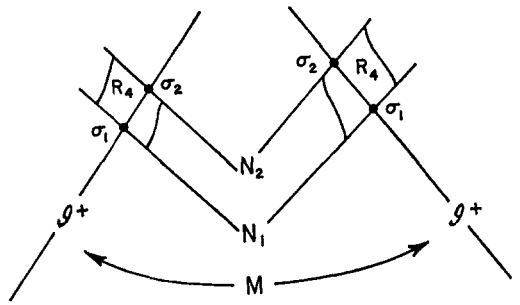


FIG. 2. R_4 is the four-dimensional region bounded by the null surfaces N_1 and N_2 which intersect $\mathfrak{I}^+$ in the two-surfaces σ_1 and σ_2. The spinor o^A is the tangent spinor to the null surfaces.

rules

$$\rho' = (\chi\bar{\chi})^{-1}\rho, \quad \pi' = \chi(\bar{\chi})^{-1}\pi,$$
$$\epsilon' = -\chi^{-2}(\bar{\chi})^{-1}D\chi + (\chi\bar{\chi})^{-1}\epsilon, \quad \sigma' = \bar{\chi}\chi^{-3}\sigma,$$
$$\alpha' = (\bar{\chi})^{-1}\chi\alpha - (\bar{\chi})^{-1}\bar{\delta}\chi, \quad \beta' = (\chi)^{-1}\bar{\chi}\beta - \bar{\chi}\chi^{-2}\delta x. \tag{6.7}$$

Accordingly,

$$\mathfrak{D}'\Phi_0' = \chi^{-(2s+1)}\bar{\chi}^{-1}\mathfrak{D}\Phi_0. \tag{6.8}$$

Hence, if $\mathfrak{W}' = \chi^{2s}\mathfrak{W}$, the conserved quantities are invariant under such scale changes. In the preceding calculations the scale was fixed so that, at $\mathfrak{I}^+$,

$$o^A\bar{o}^{\dot{X}}\nabla_{A\dot{X}}R = 1. \tag{6.9}$$

In order to investigate the conformal properties of the integrals given by (6.5), we shall consider the conformal mapping

$$g'_{\mu\nu} = f^2 g_{\mu\nu}, \tag{6.10}$$

where

$$\Omega' \equiv fR = 0$$

and

$$\nabla_\mu\Omega' \neq 0 \quad \text{at} \quad \mathfrak{I}^+. \tag{6.11}$$

In order that (6.9) be conformally invariant, the dyad spinors must transform according to the rule[18]

$$o'_A = o_A, \quad \iota'_A = \iota_A. \tag{6.12}$$

Under this transformation

$$\rho' = \frac{1}{f}\rho - \frac{1}{f^2}Df, \qquad \alpha' = \frac{1}{f}\alpha - \frac{1}{2}\frac{\delta f}{f^2},$$
$$\epsilon' = \frac{1}{f}\epsilon + \frac{1}{2}\frac{1}{f^2}Df, \qquad \beta' = \frac{1}{f}\beta + \frac{1}{f^2}\delta f, \tag{6.13}$$
$$\pi' = \frac{1}{f}\pi + \frac{\delta f}{f^2}, \qquad \sigma' = f^{-1}\sigma,$$
$$\mathfrak{D}'\Phi_0' = f^{-(s+2)}\mathfrak{D}\Phi_0, \qquad dS' = f^2\,dS.$$

Since $\alpha = \beta = 0$ at $\mathfrak{I}^+$, the analytic functions $\mathfrak{W}$ satisfy the equation at $\mathfrak{I}^+$:

$$[\bar{\delta} + (\alpha - \bar{\beta})s]\mathfrak{W} = 0. \tag{6.14}$$

[18] J. Winicour, J. Math. Phys. 9, 861 (1968).

When

$$\mathfrak{W}' = f^s\mathfrak{W}, \tag{6.15}$$

Eqs. (6.5) and (6.15) are conformally invariant.

When $f = P^{-1}$, the integrals are performed over the unit sphere at null infinity and (6.14) may be written as

$$\bar{\delta}\mathfrak{W}' = 0.$$

Consequently, in this conformal frame, the functions $\mathfrak{W}$ may be identified as the spin-weighted spherical harmonics ${}_s\bar{Y}_{sm}$.

In order to obtain a realization of $C_{s,m}$ in terms of fields in physical space–time, we recall that if the dyad in physical space–time is defined by

$$\tilde{o}^A = \Omega^{\frac{1}{2}}o^A, \quad \tilde{\iota}^A = \Omega^{-\frac{1}{2}}\iota^A, \tag{6.16}$$

the physical components of the fields peel.[8] Indeed, if Φ_0 is C^N differentiable at $\mathfrak{I}^+$, $\tilde{\Phi}_0$ can be expanded as in (4.19) where r^{-1} is now the inverse luminosity parameter Ω.

Then, since

$$\tilde{\rho} = \Omega^2\rho + \Omega D\Omega, \quad \tilde{\epsilon} = \Omega^2\epsilon, \tag{6.17}$$

it follows that

$$\mathfrak{D}\Phi_0 = \Omega^{-(2s+3)}\widetilde{\mathfrak{D}\Phi}_0 = -\tilde{\Phi}_0^1 + O(\Omega). \tag{6.18}$$

Consequently, the constants $C_{s,m}$ are, up to numerical factors, the N.P. constants in the physical manifold,

$$\int {}_s\bar{Y}_{s,m}\tilde{\Phi}_0^1\,dS. \tag{6.19}$$

Once again the invariant transformations which the quantities generate may be identified by constructing the appropriate Noether equations. For example, for the Maxwell field

$$(-\tilde{g})^{\frac{1}{2}}\tilde{A}^B{}_{\dot{X}}\tilde{\nabla}^{A\dot{X}}\tilde{\Phi}_{AB} = -\partial_{A\dot{X}}[(-g)^{\frac{1}{2}}(\tfrac{1}{2}t_{(1)}^{A\dot{X}} - H^{AB}\nabla^{C\dot{X}}\Phi_{BC})], \tag{6.20}$$

where

$$\tilde{A}^B{}_{\dot{X}} = R\nabla_{A\dot{X}}H^{AB} \tag{6.21}$$

is the potential of a Maxwell field in physical space–time, which corresponds to the Maxwell field in conformal space, whose Hertz potential H^{AB} satisfies

$$\boxtimes H^{AB} = 0.$$

For the vacuum gravitational field, there are no potentials. However, we may again construct an identity in the field variables:

$$(-\tilde{g})^{\frac{1}{2}}\tilde{A}^{BC\dot{X}\dot{Y}}\tilde{G}_{BC\dot{X}\dot{Y}} = \partial_{A\dot{X}}[(-\tilde{g})^{\frac{1}{2}}\tilde{\nabla}^D{}_{\dot{Y}}\tilde{G}_{BC}{}^{\dot{X}\dot{Y}}H^{ABC}{}_D + \tfrac{1}{2}(-g)^{\frac{1}{2}}t_{(2)}^{A\dot{X}} + (-\tilde{g})^{\frac{1}{2}}\tilde{G}_{BC}{}^{\dot{X}\dot{Y}}\nabla_{D\dot{Y}}H^{ABCD}], \tag{6.22}$$

where

$$\tilde{A}^{BC\dot{X}\dot{Y}} \equiv \tilde{\nabla}_D{}^{\dot{Y}}(\nabla_A{}^{\dot{X}} H^{ABCD}) \tag{6.23}$$

and $\boxtimes H^{ABCD} = 0$.

The Noether equations (6.20) and (6.22) give rise to the N.P. constants when the field equations are satisfied, and the spinors H^{AB} and H^{ACBD} are given by (6.1). Hence the invariant transformations which the constants generate are once again zero at all points of physical space-time and have support only on $\mathfrak{I}^+$.

7. THE EINSTEIN-MAXWELL FIELD

When the gravitational field is coupled to zero-rest-mass fields we have seen that $2(2s+1)$ constants of motion, associated with the free fields, exist. However, it appears at first sight as if the 10 gravitational quantities that are conserved when $\tilde{G}_{AB\dot{C}\dot{D}} = 0$ have no counterparts in these cases. For example, in the case of the Einstein–Maxwell fields, the natural extension of (6.22) gives

$$\begin{aligned}(-\tilde{g})^{\frac{1}{2}}\tilde{A}^{BC\dot{X}\dot{Y}}(\tilde{G}_{BC\dot{X}\dot{Y}} + \tilde{\Phi}_{BC}\tilde{\bar{\Phi}}_{\dot{X}\dot{Y}}) \\ = S + \tfrac{1}{2}\partial_{A\dot{X}}[(-g)^{\frac{1}{2}}t_{(2)}^{A\dot{X}}] \\ + \partial_{A\dot{X}}[(-\tilde{g})^{\frac{1}{2}}\tilde{\nabla}^D{}_{\dot{Y}}(\tilde{G}_{BC}{}^{\dot{X}\dot{Y}} + \Phi_{BC}\tilde{\bar{\Phi}}^{\dot{X}\dot{Y}})H^{ABC}{}_D] \\ + \partial_{A\dot{X}}[(-\tilde{g})^{\frac{1}{2}}(\tilde{G}_{BC}{}^{\dot{X}\dot{Y}} + \tilde{\Phi}_{BC}\tilde{\bar{\Phi}}^{\dot{X}\dot{Y}})\nabla_{D\dot{Y}}H^{ABCD}],\end{aligned} \tag{7.1}$$

where

$$\begin{aligned}S = H^{ABCD}\nabla_{A\dot{W}}[(-g)^{\frac{1}{2}}(\Omega^{\dot{W}\dot{Z}}\bar{\Phi}\nabla_{D\dot{Z}}\Phi_{BC} \\ + 3\bar{\Phi}^{\dot{W}\dot{Z}}\Phi_{(BC}\nabla_{D)\dot{Z}}\Omega)].\end{aligned} \tag{7.2}$$

When the gravitational field equations for these fields are satisfied,

$$\tilde{G}_{BC\dot{X}\dot{Y}} + \tilde{\Phi}_{BC}\tilde{\bar{\Phi}}_{\dot{X}\dot{Y}} = 0,$$

Eq. (7.1) gives

$$0 = \tfrac{1}{2}\partial_{A\dot{X}}[(-g)^{\frac{1}{2}}t_{(2)}^{A\dot{X}}] + S. \tag{7.3}$$

In general, expressions of this type do not lead to conservation laws. Further investigation will show, however, that in this case the Maxwell equations, constancy of charge, and the N.P. constants for the Maxwell field imply that this equation gives rise to global conservation laws.[19]

Integrating Eq. (7.3) over the region R_4 in M given by Fig. 2 and using the results of Sec. 6 gives

$$\begin{aligned}\int_{\sigma_2-\sigma_1} \mathfrak{W}\mathfrak{D}\Phi_0\, dS + 4\int_{R_3}(-g)^{\frac{1}{2}}\mathfrak{W}[\bar{\Phi}_2 D\Phi_0 \\ - \bar{\Phi}_1(\delta\Phi_0 + 2\sigma\Phi_1)]\, dV = 0,\end{aligned} \tag{7.4}$$

where $R_3 = R_4 \cap \mathfrak{I}^+$.

[19] A. Exton, E. T. Newman and R. Penrose, J. Math. Phys. **10**, 1570 (1969). A. Exton, Ph.D. thesis, University of Pittsburgh, 1967.

By using the dyad form of the Maxwell equations (4.8), together with the conditions on the standard dyad developed in Sec. 5, the integral over R_3 may be reduced to

$$\int(-g)^{\frac{1}{2}}\mathfrak{W}[\bar{\Phi}_2\mathfrak{D}\Phi_0 - \bar{\Phi}_1\mathfrak{O}\Phi_0 - 2\sigma\Phi_1\bar{\Phi}_1]\, dV, \tag{7.5}$$

where

$$\mathfrak{O}\Phi_0 \equiv (\delta + 3\bar{\pi} - 2\beta)\Phi_0 \tag{7.6}$$

and at $\mathfrak{I}^+$

$$\Delta D\Phi_0 = \bar{\delta}\mathfrak{O}\Phi_0, \tag{7.7a}$$

$$\Delta\Phi_1 = \delta\Phi_2. \tag{7.7b}$$

Under the conformal and dyad transformations (6.12) and (6.6),

$$dV' = f^{-1}\, dV, \quad dV' = \chi\bar{\chi}\, dV, \tag{7.8}$$

and the integral (7.5) is invariant. Therefore, in order to simplify the calculations and to make use of the theory of spin-weighted spherical harmonics, it is convenient to map the integral (7.5) from M to $M^{(1)}$, where the cross sections of $\mathfrak{I}^+$ are unit spheres. When this has been done, a procedure very similar to that of Ref. 19 may be followed. In order to show that the integral reduces to an expression of the same form as was calculated in those papers, it is convenient to introduce the expressions and notations used there.

We define, at $\mathfrak{I}^+$,

$$e \equiv \int_0 \bar{Y}_{00}\Phi_1\, dS, \quad = \text{const}, \tag{7.9}$$

where e is proportional to the charge ($+i \times$ magnetic charge)

$$F_m \equiv -\int_1 \bar{Y}_{1m}\mathfrak{D}\Phi_0\, dS, \quad = \text{const}, \tag{7.10}$$

where the F_m are the N.P. constants for the Maxwell field, and

$$\bar{E} \equiv \bar{e}_0 Y_{00}, \tag{7.11a}$$

$$F \equiv \sum_{m=-1}^{m=+1} F_{m\,1}Y_{1m}. \tag{7.11b}$$

Then the quantities $\bar{\delta}^{-1}(\mathfrak{D}\phi_0 - F)$ and $\bar{\delta}^{-1}(\dot{\phi}_1 - \dot{\bar{E}})$ are well defined at $\mathfrak{I}^+$ in $M^{(1)}$. It is now a straightforward matter to see that (7.5) reduces to

$$\begin{aligned}\int_{R_3} {}_2\bar{Y}_{2m}[-\bar{\Phi}_1\bar{\delta}^{-1}(\mathfrak{D}\dot{\Phi}_0 + F) \\ + \mathfrak{D}\Phi_0\bar{\delta}^{-1}(\dot{\bar{\Phi}}_0^1 - \dot{\bar{E}})](-g)^{\frac{1}{2}}\, dV,\end{aligned} \tag{7.12}$$

where the dot indicates the partial derivative Δ.

Using (7.7) again, this integral may finally be reduced to

$$\begin{aligned}-\tfrac{1}{2}\int_{\sigma_2-\sigma_1} {}_2\bar{Y}_{2m}\{(\bar{\Phi}_1 + \bar{E})\bar{\delta}^{-1}(\mathfrak{D}\Phi_0 + F) \\ - (\mathfrak{D}\Phi_0 - F)[\bar{\delta}^{-1}(\bar{\Phi}_1 - \bar{E})] + \bar{\delta}L\}\, dS.\end{aligned} \tag{7.13}$$

The term $\int {}_2\bar{Y}_{2m}\bar{\delta}L\,dS$ vanishes because L has spin weight 3.

Now the C^N differentiability of Φ_{AB} in $(M, g_{\mu\nu})$ implies that, in the physical space–time $(\tilde{M}, \tilde{g}_{\mu\nu})$,

$$\tilde{\Phi}_0 = \sum_{i=0}^{N} \frac{\tilde{\Phi}_0^i}{r^{i+3}} + O(r^{-(n+3)}), \tag{7.14}$$

$$\tilde{\Phi}_1 = \sum_{i=0}^{N} \frac{\tilde{\Phi}_1^i}{r^{i+2}} + O(r^{-(n+2)}). \tag{7.15}$$

Therefore, in physical space-time the integral expression given by (7.13) takes the form

$$\tfrac{1}{2}\int_{\sigma_2-\sigma_1} {}_2\bar{Y}_{2m}[(\tilde{\bar{\Phi}}_1^0 + \bar{E})\bar{\delta}^{-1}(\tilde{\Phi}_0^1 - F) - (\tilde{\Phi}_0^1 + F)\bar{\delta}^{-1}(\tilde{\bar{\Phi}}_1^0 - \bar{E})]\,dS. \tag{7.16}$$

Consequently (7.4) leads to the conservation law

$$\int_{\sigma_2-\sigma_1} {}_2\bar{Y}_{2m}[\tilde{\Psi}_0^1 - 2(\tilde{\bar{\Phi}}_1^0 + \bar{E})\bar{\delta}^{-1}(\tilde{\Phi}_0^1 - F) + 2(\tilde{\Phi}_0^1 + F)\bar{\delta}^{-1}(\tilde{\bar{\Phi}}_1^0 - \bar{E})]\,dS = 0. \tag{7.17}$$

This is the conservation law for the Einstein-Maxwell fields found by Exton, Newman, and Penrose.

ACKNOWLEDGMENTS

I wish to thank Dr. J. N. Goldberg for his constant encouragement and advice during the completion of this work and to acknowledge useful discussions with Dr. J. Winicour.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

One-Dimensional Bonded Fluids

G. M. BELL
Mathematics Department, Chelsea College of Science & Technology, London, England

(Received 25 November 1968)

A study is made of a linear lattice fluid in which bonds can form between pairs of molecules on second-neighbor sites with an empty site between them. At low temperatures and pressures there is, thus, competition between local open configurations and more close-packed local configurations of higher energy. By using a matrix expression for the grand partition function, the density and effective coordination number are found as functions of the absolute temperature T and one-dimensional pressure p. Equivalent results are shown to follow from a constant-pressure partition function based on an explicit expression for the configuration number. It is found that a pressure p_0 exists such that for any $p < p_0$ the open configuration is stable at $T = 0$, while the density passes through a maximum as T increases. For any $p > p_0$, on the other hand, the close-packed configuration is stable at $T = 0$ and the density decreases monotonically with T. Using a constant-pressure partition function, we also consider continuous models with the "bonding" represented by a potential well separated from the hard core. With a well of parabolic shape, similar results to those of the lattice model are obtained, while with a square well the curve of density against T displays a minimum as well as a maximum for any $p < p_0$.

1. INTRODUCTION

At pressures below about 2000 atm, curves of water density against temperature pass through a maximum, though at higher pressures the normal monotonic decrease of density with temperature is observed.[1] The qualitative explanation of the density maximum is that just above the freezing point the short-range order in water retains much of the open tetrahedrally coordinated ice structure, but that this is progressively broken down by thermal motion. The consequent closer packing over a certain range offsets the usual increase of volume with temperature. For good physical reasons, attempts to construct a statistical mechanical theory of water have usually involved models too complicated for accurate treatment.[2–5] Recently Levine and Perram,[6] by making certain simplifications and by using methods from the theory of cooperative phenomena, have been able to test some of the coordination predictions of the older theories and have discussed the possibility of phase transitions in their model.

[1] P. W. Bridgman, *The Physics of High Pressures* (G. Bell & Sons, London, 1949), Chap. 5.

[2] H. S. Frank and W. Y. Wen, Discussions Faraday Soc. **24**, 133 (1957).

[3] G. Nemethy and H. A. Scheraga, J. Chem. Phys. **36**, 3382 (1962).

[4] V. Vand and W. A. Senior, J. Chem. Phys. **43**, 1869, 1873, 1878 (1965).

[5] Y. V. Gurikuv, Zh. Strukt. Khim. **6**, 817 (1965).

[6] S. Levine and J. W. Perram, "Hydrogen-Bonded Solvent Systems," A. K. Covington and P. Jones, Eds. (Taylor and Francis Ltd., London, 1968).

The term $\int {}_2\bar{Y}_{2m}\bar{\delta}L\,dS$ vanishes because L has spin weight 3.

Now the C^N differentiability of Φ_{AB} in $(M, g_{\mu\nu})$ implies that, in the physical space–time $(\tilde{M}, \tilde{g}_{\mu\nu})$,

$$\tilde{\Phi}_0 = \sum_{i=0}^{N} \frac{\tilde{\Phi}_0^i}{r^{i+3}} + O(r^{-(n+3)}), \tag{7.14}$$

$$\tilde{\Phi}_1 = \sum_{i=0}^{N} \frac{\tilde{\Phi}_1^i}{r^{i+2}} + O(r^{-(n+2)}). \tag{7.15}$$

Therefore, in physical space-time the integral expression given by (7.13) takes the form

$$\tfrac{1}{2}\int_{\sigma_2-\sigma_1} {}_2\bar{Y}_{2m}[(\tilde{\bar{\Phi}}_1^0 + \bar{E})\bar{\delta}^{-1}(\tilde{\Phi}_0^1 - F) - (\tilde{\Phi}_0^1 + F)\bar{\delta}^{-1}(\tilde{\bar{\Phi}}_1^0 - \bar{E})]\,dS. \tag{7.16}$$

Consequently (7.4) leads to the conservation law

$$\int_{\sigma_2-\sigma_1} {}_2\bar{Y}_{2m}[\tilde{\Psi}_0^1 - 2(\tilde{\bar{\Phi}}_1^0 + \bar{E})\bar{\delta}^{-1}(\tilde{\Phi}_0^1 - F) + 2(\tilde{\Phi}_0^1 + F)\bar{\delta}^{-1}(\tilde{\bar{\Phi}}_1^0 - \bar{E})]\,dS = 0. \tag{7.17}$$

This is the conservation law for the Einstein-Maxwell fields found by Exton, Newman, and Penrose.

ACKNOWLEDGMENTS

I wish to thank Dr. J. N. Goldberg for his constant encouragement and advice during the completion of this work and to acknowledge useful discussions with Dr. J. Winicour.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

One-Dimensional Bonded Fluids

G. M. BELL
Mathematics Department, Chelsea College of Science & Technology, London, England

(Received 25 November 1968)

A study is made of a linear lattice fluid in which bonds can form between pairs of molecules on second-neighbor sites with an empty site between them. At low temperatures and pressures there is, thus, competition between local open configurations and more close-packed local configurations of higher energy. By using a matrix expression for the grand partition function, the density and effective coordination number are found as functions of the absolute temperature T and one-dimensional pressure p. Equivalent results are shown to follow from a constant-pressure partition function based on an explicit expression for the configuration number. It is found that a pressure p_0 exists such that for any $p < p_0$ the open configuration is stable at $T = 0$, while the density passes through a maximum as T increases. For any $p > p_0$, on the other hand, the close-packed configuration is stable at $T = 0$ and the density decreases monotonically with T. Using a constant-pressure partition function, we also consider continuous models with the "bonding" represented by a potential well separated from the hard core. With a well of parabolic shape, similar results to those of the lattice model are obtained, while with a square well the curve of density against T displays a minimum as well as a maximum for any $p < p_0$.

1. INTRODUCTION

At pressures below about 2000 atm, curves of water density against temperature pass through a maximum, though at higher pressures the normal monotonic decrease of density with temperature is observed.[1] The qualitative explanation of the density maximum is that just above the freezing point the short-range order in water retains much of the open tetrahedrally coordinated ice structure, but that this is progressively broken down by thermal motion. The consequent closer packing over a certain range offsets the usual increase of volume with temperature. For good physical reasons, attempts to construct a statistical mechanical theory of water have usually involved models too complicated for accurate treatment.[2–5] Recently Levine and Perram,[6] by making certain simplifications and by using methods from the theory of cooperative phenomena, have been able to test some of the coordination predictions of the older theories and have discussed the possibility of phase transitions in their model.

[1] P. W. Bridgman, *The Physics of High Pressures* (G. Bell & Sons, London, 1949), Chap. 5.

[2] H. S. Frank and W. Y. Wen, Discussions Faraday Soc. **24**, 133 (1957).

[3] G. Nemethy and H. A. Scheraga, J. Chem. Phys. **36**, 3382 (1962).

[4] V. Vand and W. A. Senior, J. Chem. Phys. **43**, 1869, 1873, 1878 (1965).

[5] Y. V. Gurikuv, Zh. Strukt. Khim. **6**, 817 (1965).

[6] S. Levine and J. W. Perram, "Hydrogen-Bonded Solvent Systems," A. K. Covington and P. Jones, Eds. (Taylor and Francis Ltd., London, 1968).

The purpose of the present paper is to consider a one-dimensional lattice and continuous fluids in which, because of the possibility of "bonding," there exist local open configurations of low energy and more close-packed configurations of higher energy. Because the models are one-dimensional, the density can be evaluated exactly as a function of pressure and temperature. It is found that, for pressures below a certain value p_0. the density passes through a maximum as the temperature increases, while above p_0 the density decreases monotonically with temperature. This behavior is similar to that of water, but since the models are physically as distant from water as a linear Ising model is from a real ferromagnet, there are, of course, qualitative differences apart from the absence of phase changes in the models. The temperature of the density maximum in the models increases with pressure, while in water it decreases.[1] Also, at intermediate pressures water density has a minimum before the maximum is attained. This occurs in one of the models, the continuous fluid with a square-well potential "bond," but at all pressures below p_0. However, the similarity between the behavior of both the lattice and continuous fluid models and that of water is sufficient to indicate that the latter is caused by simple structural factors and that the qualitative explanation given above is correct.

2. THE LATTICE FLUID

It is assumed that there is a line of N equidistantly spaced sites of which M are each occupied by a molecule m. A nearest-neighbor mm pair has an energy $-\epsilon$ ($\epsilon > 0$), while a pair of m's on second-neighbor sites can form a bond of energy $-(\epsilon + w)$, $w > 0$, if there is no m on the intervening site. If we represent such a bond by a "dash" (–), a possible configuration of 10 molecules on 20 sites, with three bonds formed, is shown in Fig. 1.

It is sometimes convenient to regard the site between a pair of bonded molecules as "occupied" by a bond b and the remaining unoccupied sites as "holes" h. The configuration of Fig. 1 is then represented as shown in Fig. 2.

If there are B bonds and H holes, then

$$M + B + H = N. \tag{2.1}$$

It should be understood that the bond energy $-(\epsilon + w)$ is not a second-neighbor energy in the ordinary sense, since a pair of m's on second-neighbor sites cannot form a bond if there is another m between them. Even if the site between the two members of the pair is empty, a bond does not necessarily exist, since the proportions of such pairs for which the bond is "formed" and "broken," respectively, depend on statistical considerations. As the system is one-dimensional, there is no long-range order except at $T = 0$, since at any absolute temperature $T > 0$ irregularities in any linear arrangement of molecules make it impossible to predict the occupation of specific sites at a macroscopic distance from a region where the occupation is known. Hence any reference to "structure" for $T > 0$ must be understood in the sense of short-range order, though the regions of short-range order may become progressively larger as T approaches zero.

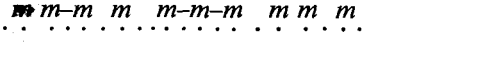


FIG. 1. Possible configuration of ten molecules on 20 sites of the linear lattice.

h m m b m h m h h m b m b m h m m h m h

FIG. 2. Alternate representation of the configuration of Fig. 1.

If N_{mm} is the number of nearest-neighbor pairs of molecules and B is the number of bonded second-neighbor pairs, then the configurational energy of the assembly is

$$E_c = -N_{mm}\epsilon - B(\epsilon + w). \tag{2.2}$$

The number of ways in which M molecules can be distributed on N sites with given values of N_{mm} and B will be denoted by $g(N, M, N_{mm}, B)$. If μ_c denotes the chemical potential, $\beta = 1/kT$ (k = Boltzmann's constant) and ϕ is the molecular partition function, assumed configuration-independent, over internal degrees of freedom, then it is useful to define

$$\lambda = \phi \exp(\beta\mu_c). \tag{2.3}$$

If the distance between neighboring sites is l_0, then the length of the assembly is equal to Nl_0. If p denotes the one-dimensional pressure, then the grand partition function is given by

$$\text{(G.P.F.)} = \exp(\beta pL) = \{\exp(\beta p l_0)\}^N = \sum_{M, N_{mm}, B} g(N, M, N_{mm}, B)\lambda^M \exp(-\beta E_c). \tag{2.4}$$

The evaluation of the (G.P.F.) will be discussed in the next section.

3. MATRIX METHOD FOR THE (G.P.F.)

For a linear assembly of several species on N sites, each configuration gives a term in the (G.P.F.) which may be written as a product of N factors,

$$A_{\alpha\beta}A_{\beta\gamma}\cdots A_{\mu\nu}\cdots A_{\omega\alpha}, \quad A_{\mu\nu} = \lambda_\mu^{\frac{1}{2}}\lambda_\nu^{\frac{1}{2}}\exp(-\beta w_{\mu\nu}), \tag{3.1}$$

where for convenience the first site is regarded as a nearest neighbor of the Nth.[7] Here λ_ν is defined for each species by an equation similar to (2.3) and $w_{\mu\nu} = w_{\nu\mu}$ is the energy of a $\mu\nu$ or $\nu\mu$ nearest-neighbor pair. For holes it is necessary to put $\lambda_h = 1$, $w_{h\nu} = 0$ (all ν). If there are n species present as well as holes, the quantities $A_{\mu\nu}$ form an $(n+1) \times (n+1)$ matrix and, assuming the $n+1$ eigenvalues are all distinct,

$$A_{\mu\nu} = \sum_{i=1}^{n+1} x_i a_i(\mu) a_i(\nu), \tag{3.2}$$

where $a_i(\nu)$ is the νth component of the normalized eigenvector $\mathbf{a}_i$, corresponding to the eigenvalue x_i. Substitution of (3.2) into (3.1) and use of the relations

$$\sum_\nu a_i(\nu) a_j(\nu) = \delta_{ij} \tag{3.3}$$

in summing over all configurations yields

$$\text{(G.P.F.)} = \sum_{i=1}^{n+1} x_i^N \sim x^N, \quad \text{for large } N, \tag{3.4}$$

where x denotes the largest eigenvalue.

This formalism can be used for the present model if it is regarded as a mixture of molecules (m), holes (h), and bonds (b), as in Fig. 2, and if

$$w_{bb} = w_{bh} = w_{hb} = \infty, \quad w_{bm} = w_{mb} = -\tfrac{1}{2}(\epsilon + w), \quad \lambda_b = 1,$$

which restricts each b to lie between two m's and gives each trio mbm the correct bond energy $-(\epsilon + w)$. The matrix A with rows and columns in order corresponding to m, h, and b is

$$A = \begin{pmatrix} \lambda y & \lambda^{\frac{1}{2}} & \lambda^{\frac{1}{2}} y^{\frac{1}{2}} z^{\frac{1}{2}} \\ \lambda^{\frac{1}{2}} & 1 & 0 \\ \lambda^{\frac{1}{2}} y^{\frac{1}{2}} z^{\frac{1}{2}} & 0 & 0 \end{pmatrix}, \tag{3.5}$$

where

$$y = \exp(\beta\epsilon), \quad z = \exp(\beta w). \tag{3.6}$$

The density ρ (number of molecules per site) is given, using (2.4) and (3.4), as

$$\rho = \frac{\bar{M}}{N} = \frac{\lambda}{N}\left(\frac{\partial \ln \text{(G.P.F.)}}{\partial \lambda}\right)_{T,N} = \frac{\lambda}{x}\Big/\left(\frac{\partial \lambda}{\partial x}\right)_T. \tag{3.7}$$

Comparing the third member of (2.4) with (3.4), we obtain

$$x = \exp(\beta p l_0), \tag{3.8}$$

and since ρ as a function of T at constant pressure is required, it is more convenient to regard x as an independent variable than λ. Since x is an eigenvalue of matrix A, given by (3.5), it satisfies the equation

$$|A - xI| = 0, \tag{3.9}$$

where I is the unit 3×3 matrix. From (3.9) it is easy to show that

$$\lambda = x^2(x-1)/\{(x-1)y(x+z) + x\}, \tag{3.10}$$

and (3.7) then gives ρ as a function of p and T in the form

$$\rho = 1 - \{x^2 + (x-1)^2 yz\}/\{(x-1)^2 y(2z+x) + x(2x-1)\}. \tag{3.11}$$

Alternatively, (3.1) may be summed over the configurations in which one particular site is occupied by ν. Substituting from (3.2) and dividing by the (G.P.F.), the mean number $\bar{N}_\nu$ of series ν is given by

$$\bar{N}_\nu/N = \sum_{i=1}^{n+1} x_i^N a_i^2(\nu) \Big/ \sum_{i=1}^{n+1} x_i^N \sim a^2(\nu), \quad \text{for large } N, \tag{3.12}$$

where $\mathbf{a}$ is the normalized eigenvector corresponding to the largest eigenvalue x of matrix A.[7] Since $\mathbf{a}$ satisfies the relation

$$(A - xI)\mathbf{a} = 0, \tag{3.13}$$

the m, h, and b components of $\mathbf{a}$ satisfy

$$a(m):a(h):a(b) = (x-1)x : x\lambda^{\frac{1}{2}} : (x-1)\lambda^{\frac{1}{2}} y^{\frac{1}{2}} z^{\frac{1}{2}}. \tag{3.14}$$

Now applying (3.12) to the mixture of m, h, and b,

$$\bar{M}/N = a^2(m), \quad \bar{H}/N = a^2(h), \quad \bar{B}/N = a^2(b). \tag{3.15}$$

From (3.14), (3.15), and the normalization condition for $\mathbf{a}$, it is easy to reproduce (3.11) and, in addition,

$$\bar{B}/N = a^2(b)\bar{M}/a^2(m)N = \lambda yz\rho/x^2, \tag{3.16}$$

with λ given by (3.10).

By summing (3.1) over configurations in which two particular sites at qth-neighbor distances are occupied by μ and ν, respectively, it is not difficult to show that, for large N, the probability is

$$\bar{N}_{\mu\nu}^{(q)}/N = a(\mu)(A^q)_{\mu\nu} a(\nu)/x^q, \tag{3.17}$$

where $\bar{N}_{\mu\nu}^{(q)}$ denotes the number of qth-neighbor $\mu\nu$ pairs. Putting $q = 1$, $\mu = \nu = m$, this gives the mean number of nearest-neighbor pairs of molecules. Using the first relation of (3.15) and (3.5),

$$\bar{N}_{mm}/N = a(m)A_{mm}a(m)/x = \lambda y \bar{M}/xN,$$

which in conjunction with (3.10) and (3.11) yields the mean effective coordination number

$$2\bar{N}_{mm}/N = 2(x-1)xy/\{(x-1)y(z+x) + x\}. \tag{3.18}$$

[7] C. Domb, Advan. Phys. **9**, 149 (1960).

Similarly,

$$\bar{N}_{mb}/N = a(m)A_{mb}a(b)/x = A_{mb}a(b)\bar{M}/Na(m)x = \lambda yz\rho/x^2. \quad (3.19)$$

Comparing (3.19) with (3.16) we see that $\bar{N}_{mb} = \bar{B}$, which verifies the consistency of the methods used.

4. CONSTANT PRESSURE PARTITION FUNCTION

An alternative method based on the explicit evaluation of the configuration number g of Sec. 2 will now be sketched. It is convenient to use the number X of hm (or of mh) nearest-neighbor pairs, rather than the number N_{mm} of mm nearest-neighbor pairs, as an independent variable. If the Nth site is regarded as a nearest neighbor of the first site, then

$$N_{mm} + X + B = M, \quad N_{hh} + X = N - M - B = H, \quad (4.1)$$

and (2.2) then becomes

$$E_c = -M\epsilon + X\epsilon - Bw. \quad (4.2)$$

We now evaluate g as a function of N, M, X, and B. First consider a distribution of M molecules and $H = N - M - B$ holes on a linear lattice of $N - B$ sites and suppose that X has its required value but $B = 0$. The number of nearest-neighbor mm pairs is now $M - X$ and the configuration number g_0 is well known (see, for instance, Ref. 8) and given by

$$g_0 = \{M!/X!\,(M - X)!\}\{H!/X!\,(H - X)!\}. \quad (4.3)$$

The bonds b must now be introduced and, since X has its required value, the only way in which the configuration can be altered to do this is to place each b between the members of one of the existing mm nearest-neighbor pairs, imagining that as each b is added, the entire distribution to the right of it shifted by a distance l_0, thus increasing the number of sites by unity. The number of ways in which the number B of bonds can be introduced is hence

$$(M - X)!/B!\,(M - X - B)! \quad (4.4)$$

and multiplication of (4.3) and (4.4) gives

$$g(N, M, X, B) = \frac{M!}{X!\,B!\,(M - X - B)!}\,\frac{(N - M - B)!}{X!\,(N - M - B - X)!}. \quad (4.5)$$

It is now possible to construct a partition function for given values of M and N and obtain a maximum term together with equilibrium values for X and B by differentiation. The maximum term can be equated to $\exp(-\beta F_c)$, where F_c is the configurational Helmholtz free energy and p is then equal to $-\partial F_c/\partial(l_0 N)$. However, it is more convenient to incorporate the pressure from the beginning by using the constant-pressure partition function Π, which is equal to $\exp(-\beta G_c)$, G_c being the configurational Gibbs free energy. The function Π is given by

$$\Pi(M, p, T) = \sum_{N,X,B} g(N, M, X, B)\exp\{-\beta(E_c + pL)\} = \sum_{N,X,B} g(N, M, X, B)x^{-N}y^{M-X}z^{B}, \quad (4.6)$$

where x is defined by (3.8) and y and z by (3.6) and Eq. (4.2) is used for E_c. By first summing over N (from $M + X + B$ to ∞) for fixed M, X, and B and then summing over B and X for all values such that $B + X \leq M$, it can be shown that

$$\Pi(M, p, T) = (x - 1)^{-1}x^{-(M-1)}[y + (x - 1)^{-1} + x^{-1}yz]^M. \quad (4.7)$$

The mean values of N, X, and B can then be obtained from

$$\bar{N} = -x\frac{\partial \ln \Pi}{\partial x}, \quad M - \bar{X} = y\frac{\partial \ln \Pi}{\partial y}, \quad \bar{B} = z\frac{\partial \ln \Pi}{\partial z}. \quad (4.8)$$

It is then easy to derive expressions for ρ, $\bar{N}_{mm} = M - \bar{X} - \bar{B}$ and $\bar{B}$, which are equivalent to (3.11), (3.18), and (3.16), respectively.

5. RESULTS FOR THE LATTICE FLUID

As $T \to 0$, $\beta \to \infty$ and, since ϵ, w, and p are all positive, the variables x, y, and z all become infinite. The equilibrium state at absolute zero depends on whether p is greater or less than the value $p_0 = w/l_0$. If $p < p_0$, then $z/x \to \infty$ as $T \to 0$, and from (3.11), (3.16), and (3.18), respectively, $\rho \to \frac{1}{2}$, $\bar{B}/N \to \frac{1}{2}$, and $\bar{N}_{mm}/N \to 0$. At absolute zero, the system thus has the open structure shown in Fig. 3,

$$m\,b\,m\,b\,m\,b\,m\,b\,m\,b\,m\,b\,m\,b\,m$$

FIG. 3. Open structure on the linear lattice.

with $N = 2M$, $\bar{B} = M$, and each molecule participating in two bonds. If $p > p_0$, on the other hand, then $z/x \to 0$ as $T \to 0$ and $\rho \to 1$, $\bar{B}/N \to 0$ and $\bar{N}_{mm}/N \to 1$. The system thus has the "close-packed structure" of Fig. 4 with all sites occupied by molecules. This

$$m\,m\,m\,m\,m\,m\,m\,m\,m\,m\,m\,m\,m\,m\,m$$

FIG. 4. Close-packed structure on the linear lattice.

[8] G. S. Rushbrooke, *Statistical Mechanics* (Oxford University Press, London, 1949), Chap. 18, Sec. 5.

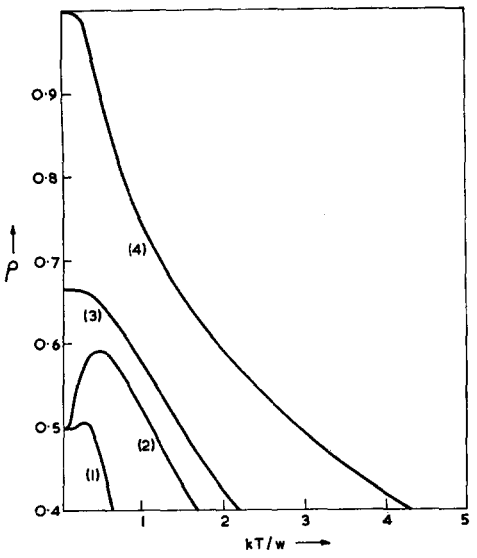


FIG. 5. Linear lattice model: density against reduced temperature for $\epsilon/w = 0$. Each curve is for a particular value of reduced pressure: (1) $pl_0/w = 0.25$, (2) $pl_0/w = 0.75$, (3) $pl_0/w = p_0l_0/w = 1$, (4) $pl_0/w = 2$.

behavior is easy to understand thermodynamically. For a given pressure the most stable state is that of minimum configurational Gibbs free energy $G_c(p, M, T)$, which reduces to the enthalpy function $H_c = E_c + pL$ at $T = 0$. Now for the open structure

$$H_c = -M(\epsilon + w) + 2pl_0M, \tag{5.1}$$

while for the close-packed structure

$$H_c = -M\epsilon + pl_0M, \tag{5.2}$$

so that the open structure has the lowest enthalpy if $p < p_0 = w/l_0$. For the case where $p = p_0$ exactly, it can be seen from (3.11) that $\rho \to \frac{2}{3}$ as $T \to 0$.

For very large T, expanding ρ in powers of $1/T$ and retaining only the leading term yields the one-dimensional perfect-gas law

$$\rho = pl_0/kT, \quad L = Nl_0 = MkT/p. \tag{5.3}$$

Since for $p > p_0$, $\rho = 1$ at $T = 0$, the density function ρ must decrease in the region just above $T = 0$. On the other hand, where $p < p_0$, it is not difficult to show from (3.11) that

$$\rho - \tfrac{1}{2} \sim \tfrac{1}{4} \exp\{-(p_0 - p)l_0/kT\}, \tag{5.4}$$

where $kT \ll w$. Since the right-hand side of (5.4) is positive and since, by (5.3), ρ must tend to zero for high T, it follows that there is at least one maximum in the curve of ρ against T for any value of $p < p_0$. Curves of ρ against the reduced temperature kT/w have been plotted numerically by using Eq. (3.11) for a number of values of ϵ/w and pl_0/w (Figs. 5 and 6), and it appears that for any $p < p_0$, the density rises to a maximum and then decreases, while for any $p > p_0$ the

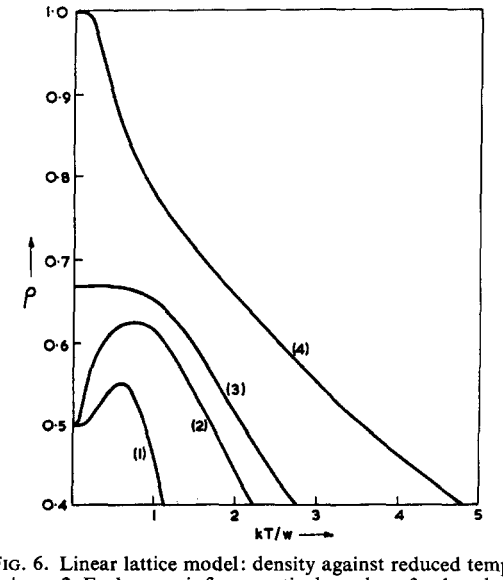


FIG. 6. Linear lattice model: density against reduced temperature for $\epsilon/w = 2$. Each curve is for a particular value of reduced pressure: (1) $pl_0/w = 0.25$, (2) $pl_0/w = 0.75$, (3) $pl_0/w = p_0l_0/w = 1$, (4) $pl_0/w = 2$.

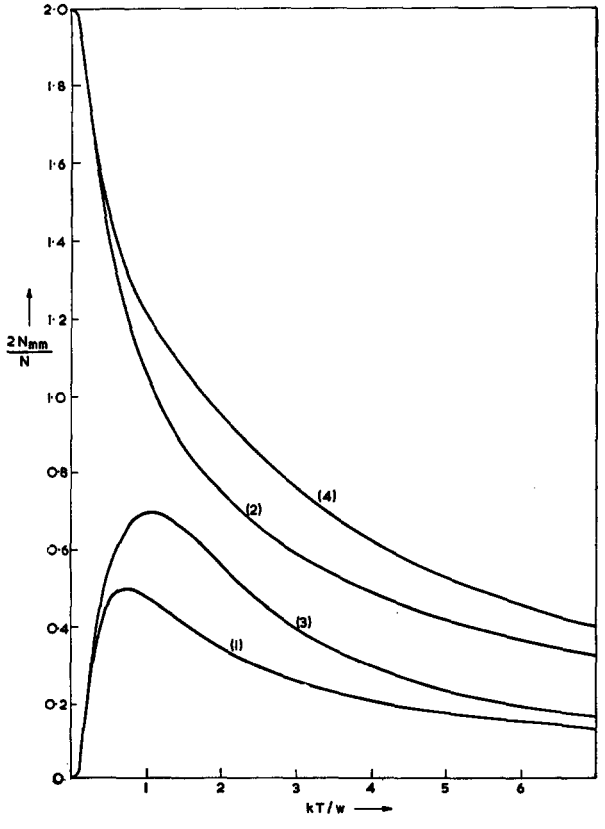


FIG. 7. Linear lattice model: mean number of first neighbors ($2N_{mm}/M$) against reduced temperature. Each curve is for a particular value of reduced pressure and of the ratio ϵ/w: (1) $pl_0/w = 0.5$, $\epsilon/w = 0$, (3) $pl_0/w = 0.5$, $\epsilon/w = 2$, (2) $pl_0/w = 1.5$, $\epsilon/w = 0$, (4) $pl_0/w = 1.5$, $\epsilon/w = 2$.

decrease is monotonic over the whole temperature range.

Equation (3.18) for $2\bar{N}_{mm}/M$ gives the mean effective coordination number or mean number of molecules on the two first-neighbor sites of a given molecule. If $p < p_0$ so that $z/x \to \infty$ as $T \to 0$, then $\bar{N}_{mm}/M \to 0$, as would be expected for the open structure. On the other hand, if $p > p_0$ so that $x/z \to \infty$ as $T \to 0$, then $\bar{N}_{mm}/M \to 1$. When T becomes very large, retention of the leading term in T^{-1} gives

$$2\bar{N}_{mm}/M \sim 2pl_0/kT \sim 2M/N, \tag{5.5}$$

the value to be expected in a random distribution. It follows that $2\bar{N}_{mm}/M$ plotted against T must have at least one maximum for any $p < p_0$. In fact, calculations for a number of values of ϵ/w and pl_0/w show that for any $p < p_0$, the curve rises to a maximum and then decreases, while for any $p > p_0$ the decrease is monotonic from the value 2 at $T = 0$ (see Fig. 7).

6. CONTINUOUS MODEL

An assembly of M molecules free to move on a segment $0 \leq x \leq L$ and with interaction energies corresponding to those of the lattice model will be considered. If a pair of molecules with centers at x_i and x_j $(x_i < x_j)$, respectively, have an interaction energy $v(x_j - x_i)$ which is such that no third molecule can lie between x_i and x_j when $v(x_j - x_i) \neq 0$, then the interaction energy V of the assembly can be written

$$V(x_1, \cdots, x_M) = \sum_{n=2}^{n=M} v(x_n - x_{n-1}), \tag{6.1}$$

where the centers are at $x_1, \cdots, x_M$, respectively, and $x_{n-1} < x_n$ for all n. The partition function is then

$$\Phi(M, L, T) = \int_0^L dx_M \int_0^{x_M} dx_{M-1} \cdots \int_0^{x_2} \exp(-\beta V)\, dx_1, \tag{6.2}$$

where a factor $M!$ allowing for permutations in the order of the molecules on the segment is cancelled with the usual factor $M!$ in the denominator. The constant pressure partition function is

$$\Pi(M, p, T) = \int_0^\infty \exp(-\beta pL)\Phi(M, L, T)\, dL. \tag{6.3}$$

It was shown by Takahashi[9] and by Gürsey[10] (see also Lieb and Mattis[11]) that an integral of the form (6.3), with Φ given by (6.1) and (6.2), can be treated as the Laplace transform of an $(M + 1)$-fold convolution so that

$$\Pi(M, p, T) = (\beta p)^{-2}\phi^{M-1}(p, T), \tag{6.4}$$

where

$$\phi(p, T) = \int_0^\infty \exp[-\beta\{v(R) + pR\}]\, dR. \tag{6.5}$$

The mean length $\bar{l}$ per molecule is given by

$$\bar{l} = \bar{L}/M = -(M\beta)^{-1}\partial \ln \Pi/\partial p = -\beta^{-1}\partial \ln \phi/\partial p. \tag{6.6}$$

Since M is regarded as very large, the factor $(\beta p)^{-2}$ in (6.4) has been neglected and the index $M - 1$ replaced by M in deriving the last expression of (6.6).

It is now necessary to specify the form of the interaction energy $v(R)$ for two molecules with centers at distance R. If the hard core of a molecule is of dimension a, it is convenient to introduce $r = R - a$ and write

$$\begin{aligned} &v(r + a) = \infty, \quad -a < r < 0, \\ &v(r + a) = 0, \quad 0 < r < r_0 - \Delta, \quad r_0 + \Delta < r, \\ &v(r + a) < 0, \quad r_0 - \Delta < r < r_0 + \Delta < a. \end{aligned} \tag{6.7}$$

There is thus a potential well in the region $r_0 - \Delta < r < r_0 + \Delta$ which is separated by a finite distance $r_0 - \Delta$ from the hard core and which corresponds to the bonding possible between second neighbors in the lattice model. The condition $r_0 + \Delta < a$ ensures that no third molecule can lie between a pair whose interaction energy is nonzero. With this form of interaction energy,

$$\phi(p, T) = (\beta p)^{-1} \exp(-\beta pa)\phi^*(p, T), \tag{6.8}$$

$$\phi^*(p, T) = 1 + \beta p \int_{r_0-\Delta}^{r_0+\Delta} \exp(-\beta pr) \times [\exp\{-\beta v(r + a)\} - 1]\, dr, \tag{6.9}$$

where clearly ϕ^* would reduce to 1 were the potential well absent. Equation (6.6) for the mean length per molecule now becomes

$$\bar{l} - a = \left[1 + \beta p \int_{r_0-\Delta}^{r_0+\Delta} r \exp(-\beta pr) \times [\exp\{-\beta v(r + a)\} - 1]\, dr\right] \Big/ \beta p\phi^*, \tag{6.10}$$

which in the absence of the potential well reduces to

$$\bar{l} - a = (\beta p)^{-1}, \tag{6.11}$$

the correct expression with a hard core potential only.[11] As $T \to \infty$ and $\beta \to 0$, Eq. (6.11) again applies

[9] H. Takahashi, Proc. Phys. Math. Soc. Japan **24**, 60 (1942). Also Ref. 11, p. 25.

[10] F. Gürsey, Proc. Cambridge Phil. Soc. **46**, 182 (1950).

[11] E. H. Lieb and D. C. Mattis, *Mathematical Physics in One Dimension* (Academic Press Inc., New York, 1966).

if the well potential is of finite magnitude, which will always be assumed.

To discuss the situation when $T \to 0$ and $\beta \to \infty$, it is useful to denote by r_m the value of r at which the sum $v(r + a) + pr$ attains its least value in the interval $r_0 - \Delta \leq r \leq r_0 + \Delta$. The point r_m may lie either at a boundary of the well (as in the square-well model of Sec. 7) or where

$$\frac{dv(r + a)}{dr} + p = 0, \quad \frac{d^2v(r + a)}{dr^2} > 0 \qquad (6.12)$$

(as in the parabolic-well model of Sec. 7). The behavior at absolute zero depends on the sign of $v(r_m + a) + pr_m$. If this is positive (as always for sufficiently large p),then both ϕ^* and the denominator of (6.10) tend to unity as $T \to 0$ and then

$$\lim_{T \to 0} (\bar{l} - a) = 0. \qquad (6.13)$$

On the other hand, if $v(r_m + a) + pr_m < 0$, the integrals in ϕ^* and (6.10) both tend to infinity with β and

$$\lim_{T \to 0} (\bar{l} - a) = r_m. \qquad (6.14)$$

The relations (6.14) and (6.13) represent, respectively, the open and close-packed structures at $T = 0$ and can be given a similar thermodynamic interpretation to that of Sec. 5. From the above considerations the pressure p_0, such that for $p > p_0$ the close-packed structure is stable at $T = 0$ and for $p < p_0$ the open structure is stable, is given by the implicit relation

$$v(r_{m0} + a) + p_0 r_{m0} = 0, \qquad (6.15)$$

r_{m0} being the value of r_m at $p = p_0$.

Finally, it is useful to define the linear density ρ by

$$\rho = a/\bar{l}. \qquad (6.16)$$

Hence $\rho = 1$ in the condensed structure at $T = 0$ and $\rho = a/(a + r_m)$ in the open structure.

7. CONTINUOUS MODEL: PARTICULAR CASES AND RESULTS

Square-Well Potential

If $v(r + a) = -v_0$, where $v_0 = \text{const} > 0$, for $r_0 - \Delta \leq r \leq r_0 + \Delta$, then, from (6.9),

$$\phi^*(p, T) = 1 + 2\{\exp(\beta v_0) - 1\} \times \exp(-\beta p r_0) \sinh(\beta p \Delta) \qquad (7.1)$$

and, from (6.10),

$$\bar{l} - a = [1 + 2\{\exp(\beta v_0) - 1\} \exp(-\beta p r_0) \times \{(1 + \beta p r_0) \sinh(\beta p \Delta) - \beta p \Delta \cosh(\beta p \Delta)\}]/\beta p \phi^*. \qquad (7.2)$$

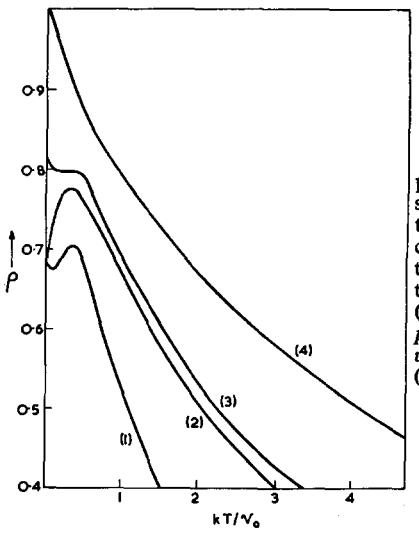


FIG. 8. Square-well potential model: density against reduced temperature. Each curve is for a particular value of the reduced pressure: (1) $pr_0/v_0 = \frac{1}{2}$, (2) $pr_0/v_0 = 1$, (3) $pr_0/v_0 = \frac{10}{9} = p_0 r_0/v_0$, (4) $pr_0/v_0 = 2$.

It can be seen from (7.1) and (7.2) that if

$$p_0 = v_0/(r_0 - \Delta), \qquad (7.3)$$

then, for $p < p_0$, $\bar{l} - a \to r_0 - \Delta$ as $T \to 0$ while, for $p > p_0$, $\bar{l} - a \to 0$ as $T \to 0$. This agrees with the arguments of Sec. 6 since, for the square-well potential, $r_m = r_0 - \Delta$ at all values of p, so that

$$v(r_m + a) + pr_m = p(r_0 - \Delta) - v_0$$

and equating this expression to zero yields (7.3). It should be noted that, if the square well is adjacent to the hard core ($r_0 = \Delta$), then $r_m = 0$ and $\bar{l} - a \to 0$ as $T \to 0$ for all values of p.

The density function ρ defined by (6.16) has been calculated from (7.1) and (7.2) as a function of the reduced temperature kT/v_0 for $\Delta/r_0 = \frac{1}{10}$, $r_0/a = \frac{1}{2}$ and several values of the reduced pressure pr_0/v_0. Some curves are shown in Fig. 8. For $p > p_0 = 10v_0/9r_0$, ρ decreases monotonically from its value of 1 at $T = 0$, while for $p < p_0$ there is a maximum. However, instead of rising directly to this maximum from its $T = 0$ value of $a/(a + r_0 - \Delta)$, the function ρ first decreases and passes through a minimum, resembling the behavior of water density at intermediate pressures.

Parabolic-Well Potential

This is defined by

$$v(r + a) = -v_0 + v_0(r - r_0)^2/\Delta^2, \quad r_0 - \Delta < r < r_0 + \Delta, \qquad (7.4)$$

so that $v(r + a)$ is continuous at the well boundaries

$r = r_0 \pm \Delta$. Substitution in (6.9) gives, where $\frac{1}{2}p\Delta/v_0 < 1$,

$$\begin{aligned}\phi^* = 1 &- 2\exp(-\beta p r_0)\sinh\beta p\Delta \\ &+ \tfrac{1}{2}\exp\{\beta(v_0 - pr_0 + \tfrac{1}{4}p^2\Delta^2/v_0)\} \\ &\times (\pi/\beta v_0)^{\frac{1}{2}}\beta p\Delta[\operatorname{erf}\{(\beta v_0)^{\frac{1}{2}}(1 + \tfrac{1}{2}p\Delta/v_0)\} \\ &+ \operatorname{erf}\{(\beta v_0)^{\frac{1}{2}}(1 - \tfrac{1}{2}p\Delta/v_0)\}]. \qquad (7.5)\end{aligned}$$

Where $\frac{1}{2}p\Delta/v_0 > 1$, the second error function in (7.5) must be changed to $-\operatorname{erf}\{(\beta v_0)^{\frac{1}{2}}(\frac{1}{2}p\Delta/v_0 - 1)\}$. It can be shown from (6.10) that

$$\begin{aligned}\bar{l} - a = r_0 &- \tfrac{1}{2}p\Delta^2/v_0 \\ &- [\beta p\{r_0 - \tfrac{1}{2}p\Delta^2/v_0 - 2\Delta\exp(-\beta p r_0) \\ &\times \cosh(\beta p\Delta)\} - 1 + 2\exp(-\beta p r_0) \\ &\times \sinh(\beta p\Delta)]/\beta p\phi^*. \qquad (7.6)\end{aligned}$$

From (7.5) and (7.6) it can be seen that, if

$$v_0 - pr_0 + \tfrac{1}{4}p^2\Delta^2/v_0 > 0, \quad v_0 > \tfrac{1}{2}p\Delta, \qquad (7.7)$$

then

$$\lim_{T\to 0}(\bar{l} - a) = r_0 - \tfrac{1}{2}p\Delta^2/r_0, \qquad (7.8)$$

but otherwise $\bar{l} - a \to 0$ as $T \to 0$. The conditions (7.7) are first broken at the lower root of the equation $v_0 - pr_0 + \frac{1}{4}p^2\Delta^2/v_0 = 0$, so that

$$p_0 = (2v_0/\Delta^2)\{r_0 - (r_0^2 - \Delta^2)^{\frac{1}{2}}\}, \qquad (7.9)$$

which is approximately v_0/r_0 for small values of Δ/r_0. At $T = 0$ it can be seen from (7.8) and (7.9) that $\bar{l} - a$ decreases from r_0 at $p = 0$ to $(r_0^2 - \Delta^2)^{\frac{1}{2}}$ at $p = p_0$. Hence as p passes through the value p_0 at $T = 0$, there is a discontinuity in $\bar{l}$ since, for $p > p_0$, $\bar{l} - a = 0$. The discontinuity disappears if the parabolic well is adjacent to the hard core ($r_0 = \Delta$).

The behavior of the system at $T = 0$ can also be deduced from the considerations of Sec. 6. For small p, the minimum value of $v(r + a) + pr$ is given by

$$\begin{aligned}dv(r_m + a)/dr_m + p &= p + (2v_0/\Delta^2)(r_m - r_0) \\ &= 0, \qquad (7.10)\end{aligned}$$

so that the right-hand side of (7.8) is r_m. Then

$$\begin{aligned}v(r_m + a) + pr_m &= -v_0 + v_0(r_m - r_0)^2/\Delta^2 + pr_m \\ &= -v_0 + pr_0 - \tfrac{1}{4}p^2\Delta^2/v_0,\end{aligned}$$

so that the first member of (7.7) represents the condition for negative $v(r_m + a) + pr_m$. Where $p = 2v_0/\Delta > p_0$, $r_m = r_0 - \Delta$ and for $p > 2v_0/\Delta$, the minimum value of $v(r + a) + pr$ is no longer given by (7.10) but always occurs at $r = r_0 - \Delta$. Hence for all $p > p_0$, $v(r_m + a) + pr_m$ is positive.

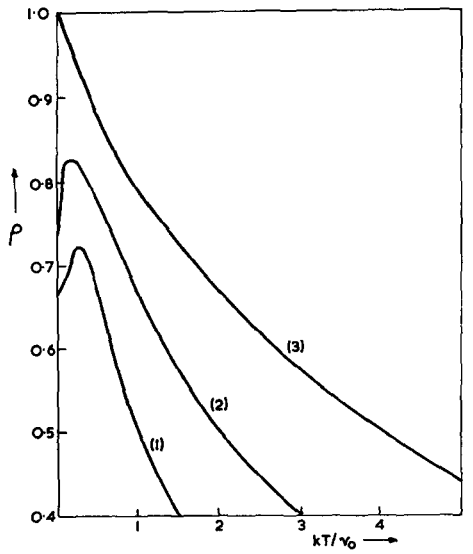


FIG. 9. Parabolic-well potential model: density against reduced temperature. Each curve is for a particular value of the reduced pressure: (1) $pr_0/v_0 = \frac{1}{2}$, (2) $pr_0/v_0 = 1$, (3) $pr_0/v_0 = 2$.

Where T is very small and β very large, it is not difficult to show from (7.5) and (7.6) that for $p < p_0$,

$$\begin{aligned}\bar{l} - a - (r_0 - \tfrac{1}{2}p\Delta^2/v_0) &\sim -(r_0 - \tfrac{1}{2}p\Delta^2/v_0) \\ &\times \exp[-\beta\{v_0 - pr_0 + \tfrac{1}{4}p^2\Delta^2/v_0\}]/\{p\Delta(\pi\beta/v_0)^{\frac{1}{2}}\}. \\ &\qquad (7.11)\end{aligned}$$

It follows that just above $T = 0$, $\bar{l}$ is smaller than its zero-point value and hence ρ [as defined by (6.16)] is larger. Hence, for $p < p_0$ the function ρ must have at least one maximum when plotted against T at constant p. By using (7.5) and (7.6), ρ has been calculated and plotted against the reduced temperature kT/v_0 for $\Delta/r_0 = \frac{1}{10}$ and several values of the reduced pressure pr_0/v_0. Where $p > p_0$, the density decreases monotonically from its value of 1 at $\bar{l} = 0$, but for $p < p_0$ it first passes through a single maximum and then decreases (Fig. 9). The behavior of the parabolic-well continuous model is thus closer to that of the lattice model than that of the square-well continuous model.

ACKNOWLEDGMENT

It is a pleasure to acknowledge the help of H. Legge (Chelsea College Computer Unit), who performed the computations.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Reduced Density Matrices of Energy Eigenstates

MITJA ROSINA
Nuclear Institute "J. Stefan" and University of Ljubljana, Ljubljana, Yugoslavia

JEROME K. PERCUS*
Courant Institute of Mathematical Sciences and Department of Physics, New York University, New York

LOUIS J. KIJEWSKI
Physics Department, Monmouth College, West Long Branch, New Jersey

AND

CLAUDE GARROD*
Physics Department, University of California, Davis, California

(Received 7 April 1969)

The following question is considered: What special properties are possessed by those reduced density matrices which come from energy eigenstates? Using the fact that $\langle\phi[H, A] \mid \phi\rangle = 0$, where A is any operator and $|\phi\rangle$ an energy eigenstate, it is shown that the elements of the two-particle density matrix are severely restricted by homogeneous linear relations. Their full content is expressed in terms of an auxiliary one-particle density which possesses additional positivity properties in the ground state.

The mathematical properties of reduced density matrices have already received extensive study (see Ref. 1 for a complete review and bibliography). In this paper we shall focus our attention on a question which appears to have been completely overlooked in the past. The question is: *What special properties are possessed by those reduced density matrices which come from the eigenstates of a given Hamiltonian?*

We consider an N-particle system of fermions or bosons with a Hamiltonian of the form

$$H = \int T(x', x)\psi^+(x')\psi(x)\, dx\, dx' + \tfrac{1}{2}\int V(x', y', x, y) \times \psi^+(y')\psi^+(x')\psi(x)\psi(y)\, dx\, dy\, dx'\, dy'. \quad (1)$$

The one- and two-body density matrices are defined by

$$\gamma(x, x') = \langle\phi|\, \psi^+(x')\psi(x)\, |\phi\rangle, \quad (2)$$

$$\Gamma(x, y, x', y') = \langle\phi|\, \psi^+(y')\psi^+(x')\psi(x)\psi(y)\, |\phi\rangle. \quad (3)$$

We shall assume that ϕ is an energy eigenstate

$$H\,|\phi\rangle = E\,|\phi\rangle. \quad (4)$$

From this, it is very easy to see that

$$\langle\phi|\, [H, A]\, |\phi\rangle = 0, \quad (5)$$

where A is any operator. In fact, the demand that Eq. (5) be satisfied for every operator A is equivalent to the statement that $|\phi\rangle$ is an energy eigenstate.

In order to obtain information about γ and Γ from Eq. (5), we choose the following special form for A:

$$A = \psi^+(z)\psi(z'). \quad (6)$$

The commutator $[H, A]$ is then given by

$$[H, A] = \int T(x', z)\psi^+(x')\psi(z')\, dx' - \int T(z', x)\psi^+(z)\psi(x)\, dx + \int V(x', y', x, z) \times \psi^+(y')\psi^+(x')\psi(x)\psi(z')\, dx\, dx'\, dy' - \int V(x', z', x, y) \times \psi^+(z)\psi^+(x')\psi(x)\psi(y)\, dx\, dy\, dx' \quad (7)$$

and its expectation becomes

$$\langle\phi|\, [H, A]\, |\phi\rangle = \int [\gamma(z', x')T(x', z) - T(z', x')\gamma(x', z)]\, dx' + \int [\Gamma(x, z', x', y')V(x', y', x, z) - V(x, z', x', y')\Gamma(x', y', x, z)]\, dx\, dx'\, dy' = 0. \quad (8)$$

Using the fact that

$$\gamma(x, x') = (N - 1)^{-1}\int \Gamma(x, y, x', y)\, dy, \quad (9)$$

we may write Eq. (8) concisely in the form

$$\int [\Gamma(x, z', x', y')h(x', y', x, z) - h(x, z', x', y')\Gamma(x', y', x, z)]\, dx\, dx'\, dy' = 0, \quad (10)$$

* Supported in part by U.S. Atomic Energy Commission, Contracts AT(30-1)-1480, AT(11-1)-Gen 10, P.A. No. 15.

[1] L. J. Kijewski and J. K. Percus, Phys. Rev. **179**, 45 (1969).

where the "reduced Hamiltonian"

$$h(x, y, x', y') \equiv (N-1)^{-1}[T(x, x')\delta(y-y') + \delta(x-x')T(y, y')] + V(x, y, x', y') \quad (11)$$

is that in which each one-body energy term is distributed among the pair energies. Indeed, h may be defined by

$$H = \tfrac{1}{2}\int h(x', y', x, y) \times \psi^+(y')\psi^+(x')\psi(x)\psi(y)\, dx\, dy\, dx'\, dy', \quad (12)$$

which replaces Eq. (1), and γ need never be introduced.

Equation (10) takes its most directly useful form in the representation in which h is diagonal. Suppose

$$h(x, y, x', y') = \sum_n \epsilon_n u_n(x, y) u_n^*(x', y'), \quad (13)$$

where the sum may actually include an integral over the continuous spectrum of h. If we express Γ in terms of the orthonormal u_n's as

$$\Gamma(x, y, x', y') = \sum_{n,m} \Gamma_{nm} u_n(x, y) u_m^*(x', y'), \quad (14)$$

then Eq. (10) states that

$$\sum_{n,m} (\epsilon_n - \epsilon_m)\Gamma_{nm} U_{nm}(z, z') = 0, \quad (15)$$

where

$$U_{nm}(z, z') \equiv \int u_n(z, y) u_m^*(z', y)\, dy.$$

One might be tempted to say that Eq. (15) indicates that Γ_{nm} vanishes whenever ϵ_n is not equal to ϵ_m. This would constitute an extremely useful result, since it would imply that Γ and h could be diagonalized together. Unfortunately, no such thing is implied by Eq. (15) because the $U_{nm}(z, z')$ are not even independent functions: (nm) is a four-particle index and (z, z') only a two-particle argument.

In order to convert Eq. (10) into a concise restriction upon the matrix elements of Γ, we will write Γ and h in the following rather unconventional representation. We first use the fact that both h and Γ are Hermitian to rewrite Eq. (10) as

$$\int [h(x', y', x, z)\Gamma^*(x', y', x, z') - \Gamma(x', y', x, z)h^*(x', y', x, z')]\, dx\, dx'\, dy' = 0. \quad (16)$$

Then we combine the one-particle variables x', y', x to form a three-particle variable $\mathbf{R}$, so that

$$\int [\Gamma^*(\mathbf{R}, z')h(\mathbf{R}, z) - h^*(\mathbf{R}, z')\Gamma(\mathbf{R}, z)]\, d^3R = 0. \quad (17)$$

Now $h(\mathbf{R}, z)$ is the kernel of a linear transformation from one-particle space ω to three-particle space Ω. It may be diagonalized in the sense that there exist two sequences of orthonormal functions $f_n(z)$ and $F_n(\mathbf{R})$ and real constants h_n, such that

$$h(\mathbf{R}, z) = \sum h_n F_n(\mathbf{R}) f_n^*(z). \quad (18)$$

We can assume that the $f_n(z)$ span ω, but the $F_n(\mathbf{R})$ can only span a linear subspace Ω' of Ω. Let us then complete the $F_n(\mathbf{R})$ to an orthonormal basis on Ω by appending the set $G_p(\mathbf{R})$, the elements of which, we note, all satisfy

$$\int h(\mathbf{R}, z) G_p^*(\mathbf{R})\, d^3R = 0. \quad (19)$$

The kernel $\Gamma(\mathbf{R}, z)$ can now be expanded in the two bases $\{f_n(z)\}$, $\{F_n(\mathbf{R})\} \cup \{G_p(\mathbf{R})\}$:

$$\Gamma(\mathbf{R}, z) = \sum P_{mn} F_m(\mathbf{R}) f_n^*(z) + \sum Q_{pn} G_p(\mathbf{R}) f_n^*(z). \quad (20)$$

Using the orthonormality properties, Eq. (17) reduces to the very simple form

$$h_m P_{mn}^* = h_n P_{nm}. \quad (21)$$

Thus $h_m P_{mn}$ is Hermitian—and $E = T_r(hP)$—but nothing can be said of Q_{pn}.

The Q_{pn} do, however, enter in describing the way in which the Hermitian matrix $h_m P_{mn}$ is also nonpositive as a matrix. Suppose that ϕ is the N-particle ground state with energy $E_0(N)$ and a is any one-body annihilator. Then clearly

$$0 \leq \langle\phi|\, a^+(H - E_0(N-1))a\, |\phi\rangle = \langle\phi|\, a^+[\{H - E_0(N-1)\}a - a\{H - E_0(N)\}]\, |\phi\rangle. \quad (22)$$

If we introduce the chemical potential

$$\mu_0(N) \equiv E_0(N) - E_0(N-1), \quad (23)$$

it follows that

$$\langle\phi|\, a^+[H, a]\, |\phi\rangle + \mu_0(N)\langle\phi|\, a^+a\, |\phi\rangle \geq 0,$$

which we write as

$$\langle\phi|\, a^+[H - \mu_0(N)\hat{N}, a]\, |\phi\rangle \geq 0, \quad (24)$$

where

$$\hat{N} \equiv \int \psi^+(x)\psi(x)\, dx.$$

On choosing $a^+ = \psi^+(z)$, $a = \psi(z')$, and evaluating (24) in the same manner as in (7), we conclude that

$$\int \{[\mu_0(N)/(N-1)]\delta(x-x')\delta(y'-z') - h(x, z', x', y')\}\Gamma(x', y', x, z)\, dx\, dx'\, dy' \quad (25)$$

is nonnegative as a matrix. To translate (25) to the

representation (18), (20), we similarly decompose

$$\delta(r_1 - r_3)\delta(r_2 - z) = \sum I_{mn}F_m(\mathbf{R})f_n^*(z) + \sum J_{pn}G_p(\mathbf{R})f_n^*(z). \quad (26)$$

It then follows at once that

$$[\mu_0(N)/(N-1)](I^+P + J^+Q)_{mn} - h_m P_{mn} \quad (27)$$

is positive semidefinite.

Equation (25) is the prototype of a number of Hamiltonian-dependent inequalities which restrict the Q_{mn} as well. For this purpose, (24) is extended to

$$\langle\phi|\,[A^+,[H,A]]\,|\phi\rangle = \langle\phi|\,A^+HA\,|\phi\rangle + \langle\phi|\,AHA^+\,|\phi\rangle \geq 0, \quad (28)$$

where A is a bilinear fermion operator. In this fashion, each of the "kinematic" inequalities of Ref. 2 gives rise to a Hamiltonian-dependent inequality. Further details can be found in Ref. 1.

ACKNOWLEDGMENT

C. Garrod and M. Rosina would like to express their appreciation to Prof. A. J. Coleman for the fine hospitality they received at Queen's University, Kingston, Ontario, where part of this work was done during the summer of 1968.

[2] C. Garrod and J. K. Percus, J. Math. Phys. 5, 1756 (1964).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Model for the Derivation of Kinetic Theory

G. V. RAMANATHAN*
Courant Institute of Mathematical Sciences, New York, New York
AND
G. SANDRI†
Aeronautical Research Associates of Princeton, Inc., Princeton, New Jersey

(Received 14 February 1969)

A soluble model for the derivation of kinetic theory is discussed. It is shown that Bogoliubov's adiabatic assumption is not valid even to leading order in the kinetic regime. Furthermore, the adiabatic assumption gives rise to a singular behavior in the correlation function which is sufficiently strong to violate the ordering assumed in the expansion. The exact result for the model correlation is neither adiabatic nor singular throughout the kinetic regime. We first show that the singularity is removed by properly reordering the correlation in the relevant domains; then a method for obtaining uniformly valid asymptotic solutions for a wide class of *integrodifferential* problems (that includes our model) is presented. We apply our technique to the BBGKY hierarchy and show that for a weakly coupled gas (i) the familiar Landau equation is satisfied in lowest order by the velocity distribution function and (ii) the two-particle correlation function can be calculated consistently to leading order, yielding a nonadiabatic and nonsingular behavior.

1. INTRODUCTION

The purpose of this paper is two-fold. One is to present a simple solvable model for kinetic theory which allows one to test the validity of various expansion techniques. The other is to develop a general method ("method of extension") for obtaining asymptotic solutions for differential and *integrodifferential* equations containing a small parameter.

The divergences that are encountered in the process of obtaining asymptotic solutions of the BBGKY hierarchy are well known.[1-5] Simple perturbation expansion in powers of the small parameter, like the density, weakness of potential, plasma parameter, etc., break down for long times because the perturbations grow with time. Such secular behavior in the first order was removed by Bogoliubov through his famous adiabatic assumption.[1] Attempts to apply the adiabatic assumption to higher orders reveal divergences which are not readily removable.[3,5]

* Work sponsored by the Air Force Office of Scientific Research, Research Grant No. AF-AFOSR-815-67.
† Work sponsored by Air Force Office of Scientific Research of the Office of Aerospace Research under Contract No. AF 49(638) 1461.

[1] N. N. Bogoliubov, *Studies in Statistical Mechanics*, J. de Boer and G. Uhlenbeck, Eds. (North-Holland Publ. Co. Amsterdam, 1962).
[2] T. Y. Wu, *Kinetic Equations of Gases and Plasmas* (Addison-Wesley Publ. Co., Reading, Mass., 1966).
[3] G. Sandri, Ann. Phys. (N.Y.) 24, 332, 380 (1963).
[4] E. A. Frieman, J. Math. Phys. 4, 410 (1963).
[5] E. G. D. Cohen and J. R. Dorfman, J. Math. Phys. 8, 282 (1967).

representation (18), (20), we similarly decompose

$$\delta(r_1 - r_3)\delta(r_2 - z) = \sum I_{mn}F_m(\mathbf{R})f_n^*(z) + \sum J_{pn}G_p(\mathbf{R})f_n^*(z). \quad (26)$$

It then follows at once that

$$[\mu_0(N)/(N-1)](I^+P + J^+Q)_{mn} - h_m P_{mn} \quad (27)$$

is positive semidefinite.

Equation (25) is the prototype of a number of Hamiltonian-dependent inequalities which restrict the Q_{mn} as well. For this purpose, (24) is extended to

$$\langle\phi|\,[A^+,[H,A]]\,|\phi\rangle = \langle\phi|\,A^+HA\,|\phi\rangle + \langle\phi|\,AHA^+\,|\phi\rangle \geq 0, \quad (28)$$

where A is a bilinear fermion operator. In this fashion, each of the "kinematic" inequalities of Ref. 2 gives rise to a Hamiltonian-dependent inequality. Further details can be found in Ref. 1.

ACKNOWLEDGMENT

C. Garrod and M. Rosina would like to express their appreciation to Prof. A. J. Coleman for the fine hospitality they received at Queen's University, Kingston, Ontario, where part of this work was done during the summer of 1968.

[2] C. Garrod and J. K. Percus, J. Math. Phys. 5, 1756 (1964).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Model for the Derivation of Kinetic Theory

G. V. RAMANATHAN*
Courant Institute of Mathematical Sciences, New York, New York
AND
G. SANDRI†
Aeronautical Research Associates of Princeton, Inc., Princeton, New Jersey

(Received 14 February 1969)

A soluble model for the derivation of kinetic theory is discussed. It is shown that Bogoliubov's adiabatic assumption is not valid even to leading order in the kinetic regime. Furthermore, the adiabatic assumption gives rise to a singular behavior in the correlation function which is sufficiently strong to violate the ordering assumed in the expansion. The exact result for the model correlation is neither adiabatic nor singular throughout the kinetic regime. We first show that the singularity is removed by properly reordering the correlation in the relevant domains; then a method for obtaining uniformly valid asymptotic solutions for a wide class of *integrodifferential* problems (that includes our model) is presented. We apply our technique to the BBGKY hierarchy and show that for a weakly coupled gas (i) the familiar Landau equation is satisfied in lowest order by the velocity distribution function and (ii) the two-particle correlation function can be calculated consistently to leading order, yielding a nonadiabatic and nonsingular behavior.

1. INTRODUCTION

The purpose of this paper is two-fold. One is to present a simple solvable model for kinetic theory which allows one to test the validity of various expansion techniques. The other is to develop a general method ("method of extension") for obtaining asymptotic solutions for differential and *integrodifferential* equations containing a small parameter.

The divergences that are encountered in the process of obtaining asymptotic solutions of the BBGKY hierarchy are well known.[1-5] Simple perturbation expansion in powers of the small parameter, like the density, weakness of potential, plasma parameter, etc., break down for long times because the perturbations grow with time. Such secular behavior in the first order was removed by Bogoliubov through his famous adiabatic assumption.[1] Attempts to apply the adiabatic assumption to higher orders reveal divergences which are not readily removable.[3,5]

* Work sponsored by the Air Force Office of Scientific Research, Research Grant No. AF-AFOSR-815-67.
† Work sponsored by Air Force Office of Scientific Research of the Office of Aerospace Research under Contract No. AF 49(638) 1461.

[1] N. N. Bogoliubov, *Studies in Statistical Mechanics*, J. de Boer and G. Uhlenbeck, Eds. (North-Holland Publ. Co. Amsterdam, 1962).
[2] T. Y. Wu, *Kinetic Equations of Gases and Plasmas* (Addison-Wesley Publ. Co., Reading, Mass., 1966).
[3] G. Sandri, Ann. Phys. (N.Y.) 24, 332, 380 (1963).
[4] E. A. Frieman, J. Math. Phys. 4, 410 (1963).
[5] E. G. D. Cohen and J. R. Dorfman, J. Math. Phys. 8, 282 (1967).

Another approach for obtaining systematic asymptotic solutions for the hierarchy is through the method of multiple time (and space) scales.[3,4,6] This method gives a rationale for Bogoliubov's assumption and yields convergent kinetic equations to the leading order. Furthermore, one obtains an expression for the rate of change of the transient part of the distribution function, which Bogoliubov's method does not give. Corrections to the leading-order collision integral have been obtained, by using multiple time and space scales, for a dilute gas.[6] For other systems, however, there seem to be divergences which cannot be removed by simple time scaling. This is most readily seen for a weakly coupled gas. For this system, without including three-body effects, the linear time scales method gives an ambiguous transient and an excessively singular correlation function in Fourier space.[7]

With a view to studying these divergences, we present in this paper a simple linear model consisting of two coupled equations. They may be looked upon as an analog of the first two equations of the hierarchy (neglecting the three-body terms) for a weakly coupled system linearized about thermal equilibrium. This model has the essential features of the equations of kinetic theory, including the singularities and secularities of the perturbation expansions. Since, by construction, three-body effects are absent in this model, any divergence arising in perturbation solution should be attributed solely to the failure of the method employed. We demonstrate that the failure of Bogoliubov's method and of the simple time-scaling method can be seen even from the leading-order results in the following sense. Although these methods give convergent collision integrals, they predict a singular behavior for the pair-correlation function in Fourier space in the leading order. Such singular behavior is spurious and can be removed by proper reordering as shown in this paper. We suggest that a substantial portion of the higher-order difficulties hinges on this spurious singularity.

Our model can be cast in the form of a single integrodifferential equation for the distribution function. The latter part of this paper is concerned with obtaining uniformly valid asymptotic solutions for such equations. We suggest a method of extension which includes the simple time scaling and Lighthill's stretching method[8] as special cases. Explicit solutions are presented for specific kernels. The convolution form of the linear integrodifferential equation presented here can be formally solved by the use of Laplace transforms. The inversion of the transform, however, is not a trivial task. The method of extension offers an alternative way of solving the equation without using transforms. Therefore, if an inversion formula can be rewritten as an integrodifferential equation, the method of extension could be used to solve it asymptotically. It should be noted that whereas the transform methods are useful only in linear problems, the method of extension does not depend on the linearity of the equation.

2. THE MODEL

The model consists of the following two equations:

$$\frac{df}{dt} = -\epsilon \int d^3x \mathbf{w} \cdot \frac{\partial U(\mathbf{x})}{\partial \mathbf{x}} g, \tag{2.1}$$

$$\frac{\partial g}{\partial t} + \mathbf{v} \cdot \frac{\partial g}{\partial \mathbf{x}} = \mathbf{w} \cdot \frac{\partial U(\mathbf{x})}{\partial \mathbf{x}} f. \tag{2.2}$$

Here f is a function of t alone, $\mathbf{v}$ and $\mathbf{w}$ are two given constant vectors, ϵ is a small positive parameter, and U a potential function dependent on $\mathbf{x}$ alone. $\mathbf{v}$ and $\mathbf{w}$ being parallel is analogous to thermal equilibrium. Then $g = Uf$. The potential U will be assumed to be a spherically symmetric function of $\mathbf{x}$. Our model can be viewed as a classical analog of the Weisskopf–Wigner model for radioactive decay.[9]

It is convenient to write these equations in Fourier space:

$$\frac{df}{dt} = +\epsilon \int d^3k (i\mathbf{k} \cdot \mathbf{w}) \tilde{U} \tilde{g}, \tag{2.3}$$

$$\frac{\partial \tilde{g}}{\partial t} + i\mathbf{k} \cdot \mathbf{v} \tilde{g} = i\mathbf{k} \cdot \mathbf{w} \tilde{U} f. \tag{2.4}$$

For simplicity, we shall assume that $\tilde{g}(0, \mathbf{k}) = 0$. We discuss below the application of standard expansion techniques to this model. Their defects are best assessed by comparison with the exact solution given in Sec. 4A for a specific interaction.

To see how the equations of the BBGKY hierarchy suggest the model equations (2.1) and (2.2), we write the equations for the one-particle distribution F^1 and for the two-particle correlation function $\Gamma \equiv F^2 - F^1F^1$ as follows:

$$\frac{\partial F^1}{\partial t} = \epsilon L \Gamma,$$

$$\frac{\partial \Gamma}{\partial t} + \mathcal{K}\Gamma = IF^1F^1 + O(\epsilon),$$

[6] E. A. Frieman and R. Goldman, J. Math. Phys. **7**, 2153 (1966); **8**, 1410 (1967).

[7] G. V. Ramanathan and G. Sandri, Bull. Am. Phys. Soc. **13**, 296 (1968).

[8] M. J. Lighthill, Phil. Mag. **7**, 40 (1949).

[9] E. Wigner and V. Weisskopf, Z. Phys. **63**, 62 (1930). A modern examination is given by M. Wellner [Phys. Rev. **118**, 875 (1960)] and a treatment based on linear time scales is given by E. Boldt and G. Sandri [Phys. Rev. **135B**, 1086 (1964)].

where we have used the operator notation of Ref. 3 (for a spatially homogeneous weakly coupled gas). The essential features of these two equations for the derivation of kinetic theory are (i) the quantities L, $\mathcal{K}$, and I are linear operators which are odd under the time-reflection transformation; (ii) the operator L is an integral operator which phase-mixes the coordinates of the typical second particle, $\mathcal{K}$ represents inertial streaming, and I represents two-body interactions; (iii) the three-body terms appear in the $O(\epsilon)$ corrections to the equation for Γ. Linearizing about equilibrium as $F^1 = F^1_{eq} + f$, $\Gamma = \Gamma_{eq} + g$, and omitting three-body effects, we find immediately that

$$\frac{\partial f}{\partial t} = \epsilon L g,$$

$$\frac{\partial g}{\partial t} + \mathcal{K} g = I f,$$

where I is an easily computed linear operator, odd under time reflection. The Eqs. (2.1) and (2.2) have the form of the linearized BBGKY equations and the three basic properties listed above. The modeling consists in replacing gradients in velocity space simply by "average eigenvalues."

For a Lorentz gas, linearization is unnecessary. Also, the equations used for the derivation of the master equation are of the form discussed above, the phase mixing occurring in higher dimensions.

Both for the BBGKY hierarchy and for our model, while the starting equations are invariant under time reflection, the kinetic approximation gives an equation that is not. It is essential for this property to hold, that L have phase-mixing properties.

A. Perturbation Theory

If we write

$$f = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \cdots,$$
$$\tilde{g} = \tilde{g}^{(0)} + \epsilon \tilde{g}^{(1)} + \epsilon^2 \tilde{g}^{(2)} + \cdots,$$

we obtain

$$\frac{df^{(0)}}{dt} = 0, \quad f^{(0)} = \text{const},$$

$$\frac{\partial \tilde{g}^{(0)}}{\partial t} + i\mathbf{k}\cdot\mathbf{v}\tilde{g}^{(0)} = i\mathbf{k}\cdot\mathbf{w}\tilde{U} f^{(0)}. \tag{2.5}$$

Upon integration, we have

$$\tilde{g}^{(0)} = \frac{\mathbf{k}\cdot\mathbf{w}}{\mathbf{k}\cdot\mathbf{v}} \tilde{U} f^0 (1 - e^{-i\mathbf{k}\cdot\mathbf{v}t}). \tag{2.6}$$

Substituting (2.6) into the equation for $f^{(1)}$, we have

$$\frac{df^{(1)}}{dt} = i f^{(0)} \int d^3k \frac{(\mathbf{k}\cdot\mathbf{w})^2}{\mathbf{k}\cdot\mathbf{v}} \tilde{U}^2 (1 - e^{-i\mathbf{k}\cdot\mathbf{v}t}),$$

whence

$$f^{(1)} = i t f^{(0)} \int d^3k \frac{(\mathbf{k}\cdot\mathbf{w})^2}{\mathbf{k}\cdot\mathbf{v}} \tilde{U}^2 - f^0 \int d^3k \frac{(\mathbf{k}\cdot\mathbf{w})^2}{(\mathbf{k}\cdot\mathbf{v})^2} (1 - e^{-i\mathbf{k}\cdot\mathbf{v}t}) \tilde{U}^2. \tag{2.7}$$

Clearly, for $t \gtrsim 1/\epsilon$ the perturbation series breaks down.

B. Bogoliubov's Method

Bogoliubov assumes that in the kinetic regime the pair correlation depends on time only through a functional of the distribution function. The equivalent expansion for the model is the following:

$$\tilde{g} = \tilde{g}^{(0)} + \epsilon \tilde{g}^{(1)} + \epsilon^2 \tilde{g}^{(2)} + \cdots, \tag{2.8}$$

$$\frac{df}{dt} = \epsilon \int d^3k i\mathbf{k}\cdot\mathbf{w}\tilde{U} g^{(0)} + \epsilon^2 \int d^3k i\mathbf{k}\cdot\mathbf{w}\tilde{U} g^{(1)} + \cdots. \tag{2.9}$$

Equation (2.2) is written as

$$\frac{\partial \tilde{g}}{\partial f}\frac{df}{dt} + i\mathbf{k}\cdot\mathbf{v}\tilde{g} = i\mathbf{k}\cdot\mathbf{w}\tilde{U} f. \tag{2.10}$$

Substituting for df/dt from (2.9) and equating powers of ϵ, we obtain

$$\tilde{g}^0 = \frac{\mathbf{k}\cdot\mathbf{w}}{\mathbf{k}\cdot\mathbf{v}} \tilde{U} f.$$

Taking into account the "generalized molecular chaos" condition of Bogoliubov, one interprets the singularity as

$$\tilde{g}^0 = P\left(\frac{\mathbf{k}\cdot\mathbf{w}}{\mathbf{k}\cdot\mathbf{v}}\right) \tilde{U} f + \pi i \delta(\mathbf{k}\cdot\mathbf{v}) \tilde{U} f. \tag{2.11}$$

Substituting this result into Eq. (2.9), we have

$$\frac{df}{dt} = -\epsilon \pi f \int d^3k (\mathbf{k}\cdot\mathbf{w})^2 \tilde{U}^2 = -\epsilon c_1 f. \tag{2.12}$$

In the next order, by substituting (2.12) for df/dt into Eq. (2.10), one gets

$$\tilde{g}^{(1)} = -i c_1 \frac{\mathbf{k}\cdot\mathbf{w}}{(\mathbf{k}\cdot\mathbf{v})^2} \tilde{U} f. \tag{2.13}$$

The correction to df/dt obtained from (2.13) is clearly divergent. The expression for $\tilde{g}^{(0)}$ given by (2.11) has a singularity at $\mathbf{k}\cdot\mathbf{v} = 0$. This singularity becomes worse in $\tilde{g}^{(1)}$. In the expansion of $\tilde{g}$ in powers of ϵ, Eq. (2.8), it has been tacitly assumed that $\tilde{g}^{(0)}$ is of order unity. This ordering breaks down when $\mathbf{k}\cdot\mathbf{v} \sim \epsilon$. This suggests a reordering which is explained in the next section.

C. Method of Linear Time Scales

This model can be analyzed by the use of time scales in the same way as one does in kinetic theory.[2,3]

One introduces a sequence of independent times $\tau_0 = t$, $\tau_1 = \epsilon t$, $\tau_2 = \epsilon^2 t$, $\cdots$ and utilizes the resulting freedom to remove the secularities in the problem:

$$f = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \cdots,$$
$$\tilde{g} = \tilde{g}^{(0)} + \epsilon \tilde{g}^{(1)} + \epsilon^2 \tilde{g}^{(2)} + \cdots,$$
$$\frac{d}{dt} = \frac{\partial}{\partial \tau_0} + \epsilon \frac{\partial}{\partial \tau_1} + \epsilon^2 \frac{\partial}{\partial \tau_2} + \cdots.$$

Substituting these expressions into (2.3) and (2.4), to the zeroth order in ϵ, one obtains

$$\frac{\partial f^{(0)}}{\partial \tau_0} = 0 \quad \text{or} \quad f^{(0)} = f^{(0)}(\tau_1, \tau_2, \cdots),$$
$$\frac{\partial \tilde{g}^{(0)}}{\partial \tau_0} + i\mathbf{k} \cdot \mathbf{v} \tilde{g}^{(0)} = i\mathbf{k} \cdot \mathbf{w} \tilde{U} f^{(0)},$$

or, for a simple choice of initial conditions,

$$\tilde{g}^{(0)} = i\mathbf{k} \cdot \mathbf{w} \tilde{U} f^{(0)} \int_0^{\tau_0} dz e^{-i\mathbf{k} \cdot \mathbf{v} z}.$$

To the first order,

$$\frac{\partial f^{(0)}}{\partial \tau_1} + \frac{\partial f^{(1)}}{\partial \tau_0} = -f^{(0)} \int d^3k (\mathbf{k} \cdot \mathbf{w})^2 \tilde{U}^2 \int_0^{\tau_0} dz e^{-i\mathbf{k} \cdot \mathbf{v} z}. \tag{2.14}$$

We notice that the first term on the left side is independent of τ_0 and the right side remains finite as $\tau_0 \to \infty$. Therefore, to keep $f^{(1)}$ finite as $\tau_0 \to \infty$, it is necessary to set

$$\frac{\partial f^{(0)}}{\partial \tau_1} = -f^{(0)} \int d^3k (\mathbf{k} \cdot \mathbf{w})^2 \tilde{U}^2 \int_0^{\infty} dz e^{-i\mathbf{k} \cdot \mathbf{v} z} \tag{2.15}$$

or

$$\frac{\partial f^{(0)}}{\partial \tau_1} = -f^{(0)} \pi \int d^3k (\mathbf{k} \cdot \mathbf{w})^2 \tilde{U}^2 \delta(\mathbf{k} \cdot \mathbf{v}),$$

which is the same result as obtained by Bogoliubov's method. It can be seen, however, that this is not sufficient to keep $f^{(1)}$ well defined as $\tau_0 \to \infty$. Subtracting (2.15) from (2.14), we obtain

$$\frac{\partial f^{(1)}}{\partial \tau_0} = -f^{(0)} \int d^3k (\mathbf{k} \cdot \mathbf{w})^2 \tilde{U}^2 \int_{\tau_0}^{\infty} dz e^{-i\mathbf{k} \cdot \mathbf{v} z}$$
$$= f^{(0)} \int d^3k \frac{(\mathbf{k} \cdot \mathbf{w})^2}{i\mathbf{k} \cdot \mathbf{v}} \tilde{U}^2 e^{-i\mathbf{k} \cdot \mathbf{v} \tau_0}. \tag{2.16}$$

The resulting $f^{(1)}$ function depends sensitively on the order of integration. The correlation function to leading order is identical with Bogoliubov's and, thus, just as singular.

Two points are worth noting here. The first is that, just as in Bogoliubov's method, here too it has been tacitly assumed that $\tilde{g}^{(0)}$ is of the order unity. The second is that, as can be seen from (2.15), the long-time (τ_1) dependence of the transient is only through $f^{(0)}$. In fact, it will be shown in Sec. 4 that this need not necessarily be so and that there is not enough freedom in the simple time scales method to decouple the transients from $f^{(0)}$.

By continuing these calculations formally to higher orders, it can be readily seen that the singular behavior of $\tilde{g}$, and consequently the divergences of the perturbations of f, become worse and worse. Therefore, even before attempting to study the higher-order corrections, one should remove the divergencies and inconsistencies in the leading-order theory.

3. REORDERING

In both Bogoliubov's method and the simple time-scales method one makes use of the fact that f varies slowly while $\tilde{g}$ varies quickly. As we shall show in this section, this is significantly not true for small values of $\mathbf{k} \cdot \mathbf{v}$. For convenience, we rewrite (2.3) and (2.4):

$$\frac{df}{dt} = \epsilon \int d^3k (i\mathbf{k} \cdot \mathbf{w}) \tilde{U} \tilde{g}, \tag{2.3'}$$

$$\frac{\partial \tilde{g}}{\partial t} + i\mathbf{k} \cdot \mathbf{v} \tilde{g} = i\mathbf{k} \cdot \mathbf{w} \tilde{U} f. \tag{2.4'}$$

It is reasonable to assume that the right side of (2.4') is bounded for all $\mathbf{k}$ and t. If $\mathbf{k} \cdot \mathbf{v}$ were finite, indeed, to the leading order, we could write

$$\tilde{g} = \frac{\mathbf{k} \cdot \mathbf{w} \tilde{U} f}{\mathbf{k} \cdot \mathbf{v}} (1 - e^{-i\mathbf{k} \cdot \mathbf{v} t}).$$

If $\mathbf{k} \cdot \mathbf{v} \sim \epsilon$, however, we can no longer do that. For, setting $k_\parallel = \epsilon k'_\parallel$ ($\parallel$ refers to the component along $\mathbf{v}$),

$$\frac{df}{dt} = \epsilon^2 \int d^2k_\perp \int_{-\infty}^{\infty} dk'_\parallel (i\mathbf{k}_\perp \cdot \mathbf{w}_\perp + \epsilon i k'_\parallel w)_\parallel \tilde{U} \tilde{g}, \tag{3.1}$$

$$\frac{\partial \tilde{g}}{\partial t} + i\epsilon k'_\parallel v \tilde{g} = (i\mathbf{k}_\perp \cdot \mathbf{w}_\perp + \epsilon i k_\parallel w_\parallel) \tilde{U} f. \tag{3.2}$$

If we assume that g is of order unity and in the first approximation we neglect the second term on the right side, we get

$$\tilde{g} \sim (i\mathbf{k}_\perp \cdot \mathbf{w}_\perp) \tilde{U} f t.$$

Thus, for times of the order $1/\epsilon$, $\tilde{g}$ grows to be of the order of $1/\epsilon$. This violates our assumption that $\tilde{g} \sim 1$. To neglect $i\epsilon k'_\parallel v g$ is no longer justifiable. Therefore, for times of the order $1/\epsilon$, we have to reorder $\tilde{g}$ in the following way:

$$\tilde{g} = (1/\epsilon) \tilde{g}', \tag{3.3}$$

$$t = (1/\epsilon) t'. \tag{3.4}$$

Then (3.1) and (3.2) become

$$\frac{df}{dt'} = \int d^2k_\perp \int_{-\infty}^{\infty} dk'_\parallel (i\mathbf{k}_\perp \cdot \mathbf{w}_\perp + \epsilon i k'_\parallel w_\parallel) \tilde{U} \tilde{g}', \quad (3.5)$$

$$\frac{\partial \tilde{g}'}{\partial t'} + ik'_\parallel v \tilde{g}' = (i\mathbf{k}_\perp \cdot \mathbf{w}_\perp + i\epsilon k'_\parallel w_\parallel) \tilde{U} f. \quad (3.6)$$

Thus, we see that for small values of $k_\parallel$, $\tilde{g}$ evolves in time on the same scale as f. For long times, the region of small $k_\parallel$ is the relevant region as far as the collision integral is concerned, and it is in this region that Bogoliubov's assumption breaks down.

From (3.5) and (3.6) we can obtain the kinetic equation and the correlation function to the leading order in this region by setting $\epsilon = 0$ in these equations. Thus,

$$\frac{df}{dt'} = -\int d^2k (\mathbf{k}_\perp \cdot \mathbf{w}_\perp)^2 \tilde{U}(k_\perp) \times \int_{-\infty}^{\infty} dk_\parallel \int_0^{t'} dz e^{-ik_\parallel' vz} f(t' - z), \quad (3.5')$$

$$\tilde{g}' = (i\mathbf{k}_\perp \cdot \mathbf{w}_\perp) \tilde{U}(k_\perp) \int_0^{t'} dz e^{-ik_\parallel' vz} f(t' - z). \quad (3.6')$$

Assuming that the $k_\parallel$ and z integrations can be interchanged,

$$\frac{df}{dt'} = -\gamma f, \quad \gamma = \frac{\pi}{v} \int d^2k_\perp (\mathbf{k}_\perp \cdot \mathbf{w}_\perp)^2 \tilde{U}^2(k_\perp),$$

which coincides with the result obtained through Bogoliubov's method, if one keeps in mind (3.4). The correlation, however, is slightly different:

$$\tilde{g}' = \frac{\mathbf{k}_\perp \cdot \mathbf{w}_\perp \tilde{U}(k_\perp)}{k'v + i\gamma} (e^{-\gamma t'} - e^{-ik_\parallel' vt'}) \quad (3.7)$$

or

$$\tilde{g} = \frac{\mathbf{k}_\perp \cdot \mathbf{w}_\perp \tilde{U}}{k_\parallel v + i\epsilon\gamma} (e^{-\epsilon\gamma t} - e^{-ik_\parallel vt}). \quad (3.8)$$

This result is large for small values of $k_\parallel$, but, unlike the adiabatic result, it remains bounded. In Appendix A we do the reordering for the BBGKY equations for a weakly coupled system and derive the Fokker–Planck equation.

4. INTEGRODIFFERENTIAL EQUATION

The model can be represented by a single linear integrodifferential equation. For simplicity, we assume that initially g is zero everywhere. Solving for g and substituting in the equation for f, the following equation is obtained:

$$\frac{df}{dt} = \epsilon \int_0^t dz K(t, z) f(z), \quad (4.1)$$

where

$$K(t, z) = -\int d^3k e^{-i\mathbf{k}\cdot\mathbf{v}(t-z)} (\mathbf{k} \cdot \mathbf{w})^2 \tilde{U}^2. \quad (4.2)$$

In this section we shall develop a method for obtaining uniformly valid solutions for (4.1). We shall *not* assume that $K(t, z) = K(t - z)$ as in (4.2). The functional dependence of K on t and z can be arbitrary, subject to the conditions

$$K(t, 0) \quad \text{is bounded,}$$

$$\lim_{t\to\infty} \int_0^t dz K(t, z) \quad \text{is finite.}$$

For simplicity, we assume that K is independent of ϵ.

It can be readily seen that, in general, an expansion of f in powers of ϵ will break down for $t \sim 1/\epsilon$. To get around this difficulty, we search for a new domain in which this secular behavior would not occur. For this purpose, we embed t into a space T of dimension $N + 1$, $\{\tau_0, \tau_1, \tau_2, \cdots, \tau_N\}$. (For more details on extension, see Ref. 3. In this paper we do not attempt to answer questions concerning the mathematical rigor of this method. We merely present in an intuitive manner a possible method that could be useful in solving physical problems.) The set of points constituting the original domain will now be the line in T given by $\tau_n = T_n(t)$, $n = 0, 1, \cdots, N$. This line will be called the "physical line." The functions T_i can depend quite generally on ϵ. A function

$$\mathbf{f}\{\tau_n\} \equiv \mathbf{f}(\tau_0, \tau_1, \cdots)$$

is called an extension of $f(t)$ if and only if

$$\mathbf{f}\{T_n(t)\} = f(t). \quad (4.3)$$

It is clear from this definition that the extension of a function is not unique. For example, if $\tau_0 = T_0(t)$ has an inverse $t = t(\tau_0)$ and $\mathbf{A}\{\tau_n\}$ is a function such that $\mathbf{A}\{0\} = 0$, then the function

$$\mathbf{f}^*\{\tau_n\} = \mathbf{f}\{\tau_n\} + \mathbf{A}\{\tau_n - T_n(t(\tau_0))\}$$

is also an extension of f, if $\mathbf{f}$ is an extension of f.

Summarizing our notation,

$$\tau_n = T_n(t) \equiv T_n[\tau_0], \quad 0 \le n \le N, \quad (4.4a)$$

$$\tau_0 = T_0(t), \quad t = t(\tau_0). \quad (4.4b)$$

We now apply our definition of extension, Eq. (4.3), to the derivative and to the integral

$$\phi(t) = df/dt, \quad (4.5a)$$

$$\psi(t) = \int_0^t dt' F(t; t'). \quad (4.5b)$$

It is readily verified, using (4.3), that

$$\Phi\{\tau_n\} = \left[\frac{dt(\tau_0)}{d\tau_0}\right]^{-1} \sum_{n=0}^{N} \frac{dT_n[\tau_0]}{d\tau_0} \frac{\partial}{\partial \tau_n} \mathbf{f}\{\tau_n\}, \quad (4.6a)$$

$$\Psi\{\tau_n\} = \int_{T_0(0)}^{\tau_0} d\tau_0' \left[\frac{dt'(\tau_0')}{d\tau_0'}\right] \mathbf{F}\{\tau_n; \tau_n - T_n[\tau_0] + T_n[\tau_0']\} \quad (4.6b)$$

are extensions of ϕ and ψ, respectively. Furthermore, $\mathbf{f}$ is an extension of f if and only if Φ is an extension of ϕ, and similarly for F and ψ.

In a problem with a small parameter ϵ, the T's will be functions of ϵ. After performing the extension, we look for a solution for the extended dependent variable in powers of ϵ. We impose on this solution the condition that the terms in the power series should become successively smaller as ϵ tends to zero. We utilize the freedom resulting from the extension to remove nonuniformities in the perturbations. After obtaining a solution in the extended space, we project it onto the physical line. Without any loss of generality, we can assume that $t(\tau_0, \epsilon = 0) = \tau_0$, because any ϵ-independent transformation of t is not relevant to the asymptotic analysis of the problem. Furthermore, we shall view the sequence $\{T_n[\tau_0]\}$ as one of successively more and more slowly varying functions. Thus, the T's are expanded as follows:

$$t(\tau_0) = \tau_0 + \epsilon\xi_0(\tau_0) + \epsilon^2\eta_0(\tau_0) + \cdots, \quad (4.7)$$

$$T_1[\tau_0] = \epsilon\xi_1(\tau_0) + \epsilon^2\eta_1(\tau_0) + \cdots, \quad (4.8)$$

$$T_2[\tau_0] = \epsilon^2\eta_2(\tau_0) + \cdots, \quad (4.9)$$

and so on. The functions $\xi_0, \xi_1, \cdots, \eta_0, \eta_1, \cdots$ will have to be determined from the uniformity conditions. Setting $t = 0$ in (4.7), $T_0(0)$ can be expressed as a power series in ϵ:

$$T_0(0) = -\epsilon\xi_0(0) + \epsilon^2[\xi_0(0)\xi_0'(0) - \eta_0(0)] + \cdots. \quad (4.10)$$

Now, we extend Eq. (4.1) using (4.6) and look for a solution of the form

$$\mathbf{f} = \mathbf{f}^{(0)} + \epsilon\mathbf{f}^{(1)} + \epsilon^2\mathbf{f}^{(2)} + \cdots. \quad (4.11)$$

It is worth noting that $T_1 = T_2 = \cdots = 0$ corresponds to Lighthill's method and $t = \tau_0$, $T_i = \epsilon^i\tau_0$ corresponds to the simple time scales method.

Expanding both sides of the extended form of Eq. (4.1) in powers of ϵ and equating powers, the following equations are obtained up to the second order:

$$\frac{\partial \mathbf{f}^{(0)}}{\partial \tau_0} = 0, \quad (4.12)$$

$$\frac{d\xi_1}{d\tau_0}\frac{\partial \mathbf{f}^{(0)}}{\partial \tau_1} + \frac{\partial \mathbf{f}^{(1)}}{\partial \tau_0} = \int_0^{\tau_0} d\mu K(\tau_0, \mu)\mathbf{f}^{(0)}(\mu, \tau_1, \cdots), \quad (4.13)$$

$$\begin{aligned}
&\frac{d\eta_2}{d\tau_0}\frac{\partial \mathbf{f}^{(0)}}{\partial \tau_2} + \frac{d\eta_1}{d\tau_0}\frac{\partial \mathbf{f}^{(0)}}{\partial \tau_1} + \frac{d\xi_1}{d\tau_0}\frac{\partial \mathbf{f}^{(1)}}{\partial \tau_1} + \frac{\partial \mathbf{f}^{(2)}}{\partial \tau_0} \\
&\quad = \xi_0(0)\mathbf{f}^{(0)}(0, \tau_1, \tau_2, \cdots)K(\tau_0, 0) \\
&\qquad + \int_0^{\tau_0} d\mu K(\tau_0, \mu)\mathbf{f}^{(1)}(\mu, \tau_1, \tau_2, \cdots) \\
&\qquad + \frac{d\xi_0}{d\tau_0}\int_0^{\tau_0} d\mu K(\tau_0, \mu)\mathbf{f}^{(0)}(\mu, \tau_1, \cdots) \\
&\qquad + \int_0^{\tau_0} d\mu \Bigg(\mathbf{f}^{(0)}(\mu, \tau_1, \cdots)\frac{\partial}{\partial \mu}[K(\tau_0, \mu)\xi_0(\mu)] \\
&\qquad + \mathbf{f}^{(0)}(\mu, \tau_1, \cdots)\frac{\partial K(\tau_0, \mu)}{\partial \tau_0}\xi_0(\tau_0) \\
&\qquad - \frac{\partial \mathbf{f}^{(0)}(\mu, \tau_1, \cdots)}{\partial \tau_1} K(\tau_0, \mu)[\xi_1(\tau_0) - \xi_1(\mu)] \Bigg).
\end{aligned} \quad (4.14)$$

The above equations are in a very general form. In particular, they include the terms that arise in:

(i) Simple perturbation theory (obtainable by setting $\xi_0 = \xi_1 = \eta_1 = \eta_2 = 0$),

(ii) Linear time scale theory (those containing ξ_1 and η_2),

(iii) Lighthill's method (those containing ξ_0), and

(iv) The "mixed" term containing η_1.

It may be observed that so far there are seven unknown functions, namely, $\mathbf{f}^{(0)}$, $\mathbf{f}^{(1)}$, $\mathbf{f}^{(2)}$, ξ_0, ξ_1, η_1, and η_2 related by three equations and two nonsecularity conditions, namely, $\mathbf{f}^{(1)}/\mathbf{f}^{(0)}$ should be bounded everywhere and $\mathbf{f}^{(2)}/\mathbf{f}^{(1)}$ should be bounded everywhere. We, therefore, have enough freedom to impose further restrictions on these functions. Since we should like to obtain solutions as close to the exact solution as possible, it is reasonable to impose a condition on the transients $\mathbf{f}^{(2)}$ and $\mathbf{f}^{(1)}$ that

$$\frac{\partial \mathbf{f}^{(2)}}{\partial \tau_0} \Big/ \frac{\partial \mathbf{f}^{(1)}}{\partial \tau_0}$$

be bounded everywhere. This we shall call the condition of differential uniformity.

From (4.12) we have

$$\mathbf{f}^{(0)} = \mathbf{f}^{(0)}(\tau_1, \tau_2, \cdots). \quad (4.15)$$

In the first order, noticing that $\mathbf{f}^{(0)}(\mu, \tau_1, \cdots)$ is independent of μ, Eq. (4.13) becomes

$$\frac{d\xi_1}{d\tau_0}\frac{\partial \mathbf{f}^{(0)}}{\partial \tau_1} + \frac{\partial \mathbf{f}^{(1)}}{\partial \tau_0} = \mathbf{f}^{(0)}\int_0^{\tau_0} d\mu K(\tau_0, \mu). \quad (4.16)$$

Since this should be true for all τ_0, $\partial \mathbf{f}^{(0)}/\partial\tau_1 = \gamma_1 \mathbf{f}^{(0)}$ where γ_1 is a constant, it may be observed that this constant can be absorbed into the as yet undetermined function $\xi_1(\tau_0)$. Thus, without loss of generality, we set

$$\frac{\partial \mathbf{f}^{(0)}}{\partial \tau_n} = \mathbf{f}^{(0)}, \quad n \geq 1. \tag{4.17}$$

Let us also write $\mathbf{f}^{(n)} = \mathbf{f}^{(0)}\mathbf{F}^{(n)}$. Now (4.13) and (4.14) can be written in the following form:

$$\frac{\partial \mathbf{F}^{(1)}}{\partial \tau_0} = -\frac{d\xi_1}{d\tau_0} + \int_0^{\tau_0} d\mu K(\tau_0, \mu) = G(\tau_0), \tag{4.18}$$

$$\begin{aligned}\frac{\partial \mathbf{F}^{(2)}}{\partial \tau_0} &= \int_0^{\tau_0} d\mu K(\tau_0, \mu)\mathbf{F}^{(1)}(\mu, \tau_1, \cdots) \\ &\quad + \frac{d}{d\tau_0}\left[\xi_0(\tau_0)\int_0^{\tau_0} d\mu K(\tau_0, \mu)\right] \\ &\quad - \int_0^{\tau_0} d\mu K(\tau_0, \mu)(\xi_1(\tau_0) - \xi_1(\mu)) \\ &\quad - \frac{d\eta_1}{d\tau_0} - \frac{d\eta_2}{d\tau_0} - \frac{d\xi_1}{d\tau_0}\left(\frac{\partial \mathbf{F}^{(1)}}{\partial \tau_1} + \mathbf{F}^{(1)}\right) \\ &= H(\tau_0).\end{aligned} \tag{4.19}$$

We note that G is a function of τ_0 only. We show below that H also is a function of τ_0 only. Now, the uniformity conditions are

$$\lim_{\tau_0 \to \infty} \int_0^{\tau_0} G(\lambda)\, d\lambda < M_1, \tag{4.20}$$

$$\lim_{\tau_0 \to \infty} \int_0^{\tau_0} H(\lambda)\, d\lambda < M_2, \tag{4.21}$$

$$\lim_{\tau_0 \to \infty} \frac{H(\tau_0)}{G(\tau_0)} < M_3, \tag{4.22}$$

where M_1, M_2, and M_3 are constants. Solving for $\mathbf{F}^{(1)}$ from (4.18), we have

$$\mathbf{F}^{(1)} = A(\tau_1, \tau_2, \cdots) - \xi_1(\tau_0) + \int_0^{\tau_0} d\lambda \int_0^{\lambda} d\mu K(\lambda, \mu). \tag{4.23}$$

Substituting this into (4.19), using the uniformity conditions, and noticing that A is not a function of τ_0, we have

$$\frac{\partial A}{\partial \tau_1} = \text{const} = 0.$$

The constant has to be set to zero to prevent A from growing with τ_1. Anticipating that A will be a pure constant (which follows from higher-order theory), we absorb this constant in ξ_1 and set

$$A = 0.$$

Therefore,

$$\mathbf{F}^{(1)} = -\xi_1(\tau_0) + \int_0^{\tau_0} d\lambda \int_0^{\lambda} d\mu K(\lambda, \mu). \tag{4.24}$$

Substituting (4.24) into (4.19), we obtain

$$\begin{aligned}H(\tau_0) &= \int_0^{\tau_0} d\lambda K(\tau_0, \lambda) \int_0^{\lambda} d\mu \int_0^{\mu} d\nu K(\mu, \nu) \\ &\quad + \frac{d}{d\tau_0}\left(\xi_0(\tau_0)\int_0^{\tau_0} d\mu K(\tau_0, \mu)\right) \\ &\quad - \frac{d\xi_1(\tau_0)}{d\tau_0}\int_0^{\tau_0} d\lambda \int_0^{\lambda} d\mu K(\lambda, \mu) \\ &\quad - \xi_1(\tau_0)\int_0^{\tau_0} d\mu K(\tau_0, \mu) \\ &\quad + \xi_1(\tau_0)\frac{d\xi_1(\tau_0)}{d\tau_0} - \frac{d}{d\tau_0}(\eta_1 + \eta_2).\end{aligned} \tag{4.25}$$

There is still a great deal of freedom available for the choice of the functions ξ_0, ξ_1, η_1, and η_2. Often in practice, the choice will depend on the particular problem at hand. We shall illustrate the method by considering two specific kernels, namely, an exponential and a Gaussian.

A. Exponential Kernel

Consider

$$K(t, z) = -e^{-t+z}.$$

For this kernel we find, from (4.24), that

$$\mathbf{F}^{(1)}(\tau_0) = -\xi_1(\tau_0) - \tau_0 + 1 - e^{-\tau_0}. \tag{4.26}$$

From (4.18),

$$G(\tau_0) = -\frac{d\xi_1}{d\tau_0} - 1 + e^{-\tau_0}$$

and, from (4.25),

$$\begin{aligned}H(\tau_0) &= \tau_0\left(1 + \frac{d\xi_1}{d\tau_0}\right) - 2 + 2e^{-\tau_0} \\ &\quad + \tau_0 e^{-\tau_0} - \xi_0 e^{-\tau_0} - \frac{d\xi_0}{d\tau_0}(1 - e^{-\tau_0}) \\ &\quad - \frac{d\xi_1}{d\tau_0}(1 - e^{-\tau_0}) - \xi_1 e^{-\tau_0} + \xi_1 \\ &\quad + \xi_1\frac{d\xi_1}{d\tau_0} - \frac{d}{d\tau_0}(\eta_1 + \eta_2).\end{aligned} \tag{4.27}$$

The condition (4.20) is satisfied by setting

$$\xi_1(\tau_0) = -\tau_0. \tag{4.28}$$

Then,

$$G(\tau_0) = e^{-\tau_0}$$

and

$$H(\tau_0) = -2 + 2e^{-\tau_0} + 2\tau_0 e^{-\tau_0} - \xi_0 e^{-\tau_0} - \frac{d\xi_0}{d\tau_0}(1 - e^{-\tau_0}) + (1 - e^{-\tau_0}) - \frac{d}{d\tau_0}(\eta_1 + \eta_2).$$

To satisfy the conditions (4.21) and (4.22) we choose

$$\xi_0 = 2\tau_0, \tag{4.29}$$

$$\eta_1 + \eta_2 = -3\tau_0. \tag{4.30}$$

Thus, we have

$$\mathbf{f}^{(0)} = Ce^{\tau_1+\tau_2}, \tag{4.31}$$

$$\mathbf{F}^{(1)} = 1 - e^{-\tau_0}, \tag{4.32}$$

$$\frac{\partial \mathbf{F}^{(2)}}{\partial \tau_0} = H(\tau_0) = 3e^{-\tau_0}. \tag{4.33}$$

By the same arguments as for setting $A = 0$, we shall take $\mathbf{F}^{(2)}$ $(\tau_0 = 0) = 0$, so that

$$\mathbf{F}^{(2)} = 3(1 - e^{-\tau_0}).$$

Now we project the solution onto the physical line by setting

$$\tau_1 = \epsilon\xi_1(\tau_0) + \epsilon^2\eta_1(\tau_0), \tag{4.34}$$

$$\tau_2 = \epsilon^2\eta_2(\tau_0), \tag{4.35}$$

and

$$t = \tau_0 + \epsilon\xi_0(\tau_0). \tag{4.36}$$

Substituting (4.34) and (4.35) into (4.31) and using (4.28) and (4.30), we obtain, evaluating $\mathbf{f}^{(0)}$ along the physical line,

$$f^{(0)} = Ce^{-\epsilon\tau_0 - 3\epsilon^2\tau_0}.$$

From (4.36) and (4.29),

$$\tau_0 = t(1 - 2\epsilon) + O(\epsilon^2). \tag{4.37}$$

Therefore,

$$\begin{aligned} f^{(0)} &= Ce^{-\epsilon t - \epsilon^2 t}, \\ f^{(1)} &= f^{(0)}F^{(1)} = Ce^{-\epsilon t - \epsilon^2 t}(1 - e^{-t+2\epsilon t}) \\ &= Ce^{-\epsilon t - \epsilon^2 t} - Ce^{-t+\epsilon t}, \\ f^{(2)} &= 3C(e^{-\epsilon t - \epsilon^2 t} - e^{-t+\epsilon t}). \end{aligned} \tag{4.38}$$

In Eq. (4.38), in the last term on the right-hand side, the $\epsilon^2 t$ in the exponent has been dropped since the decay-time correction to this order can only be obtained from third-order theory. Finally, combining these results, we have

$$f = f(0)(1 + \epsilon + 3\epsilon^2)e^{-\epsilon t - \epsilon^2 t} - f(0)(\epsilon + 3\epsilon^2)e^{-t+\epsilon t} + O(\epsilon^3). \tag{4.39}$$

Thus, f has a finite slowly-varying part and a small transient part.

For this kernel the integral equation can be solved exactly. The solution is

$$\begin{aligned} f &= \frac{f(0)}{(1 - 4\epsilon)^{\frac{1}{2}}}\left[\left(\frac{-1 + (1 - 4\epsilon)^{\frac{1}{2}}}{2}\right)\right. \\ &\quad \times \exp\left(\frac{-1 - (1 - 4\epsilon)^{\frac{1}{2}}}{2}t\right) \\ &\quad \left. + \left(\frac{-1 + (1 - 4\epsilon)^{\frac{1}{2}}}{2}\right)\exp\left(\frac{-1 + (1 - 4\epsilon)^{\frac{1}{2}}}{2}t\right)\right] \\ &= f(0)[(1 + \epsilon + 3\epsilon^2)e^{-\epsilon t - \epsilon^2 t} \\ &\quad - (\epsilon + 3\epsilon^2)e^{-t+\epsilon t}] + O(\epsilon^3), \end{aligned}$$

which is the same as (4.39) up to the second order. Each higher-order calculation yields a correction to the exponent as well as a correction to the amplitude.

It is worth noting that a Bogoliubov-type expansion would not give the transient, while the linear time-scales method would give the following:

$$f = f(0)e^{-\epsilon t - \epsilon^2 t}[1 + \epsilon + 3\epsilon^2 + e^{-t}(\epsilon + 3\epsilon^2 + 2\epsilon^2 t + \cdots)].$$

In other words, in the linear time scales method, the behavior of $\mathbf{f}^{(1)}$ in the slow time scale would be given as a perturbation around the behavior of $f^{(0)}$. In our more general method, there is sufficient freedom to decouple $f^{(1)}$ from $f^{(0)}$ to obtain the correct long-time behavior.

B. Gaussian Kernel

Consider

$$K(t, \lambda) = -e^{-(t-\lambda)^2/2}.$$

This kernel corresponds to a potential

$$U(x) \propto e^{-ax^2}$$

in the model. An exact solution of the integral equation cannot be obtained. For this case

$$G(\tau_0) = -\frac{d\xi_1}{d\tau_0} - \int_0^{\tau_0} d\mu e^{-\mu^2/2}, \tag{4.40}$$

$$\mathbf{F}^{(1)} = -\xi_1 - \tau_0\int_0^{\tau_0} d\mu e^{-\mu^2/2} + (1 - e^{-\tau_0^2/2}), \tag{4.41}$$

$$\begin{aligned} H(\tau_0) &= \tfrac{1}{2}\tau_0\left(\int_0^{\tau_0} d\mu e^{-\mu^2/4}\right)^2 + 2e^{-\tau_0^2/4}\int_0^{\tau_0} d\mu e^{-\mu^2/4} \\ &\quad - 2\int_0^{\tau_0} d\mu e^{-\mu^2/2} - \frac{d\xi_0}{d\tau_0}\int_0^{\tau_0} d\mu e^{-\mu^2/2} - \xi_0 e^{-\tau_0^2/2} \\ &\quad + \frac{d\xi_1}{d\tau_0}\tau_0\int_0^{\tau_0} d\mu e^{-\mu^2/2} - \frac{d\xi_1}{d\tau_0}(1 - e^{-\tau_0^2/2}) \\ &\quad + \xi_1\int_0^{\tau_0} d\mu e^{-\mu^2/2} + \xi_1(\tau_0)\frac{d\xi_1}{d\tau_0} - \frac{d}{d\tau_0}(\eta_1 + \eta_2). \end{aligned} \tag{4.42}$$

The uniformity condition (4.20) is guaranteed by setting

$$\xi_1(\tau_0) = -\tau_0\int_0^\infty d\mu e^{-\mu^2/2} = -(\pi/2)^{\frac{1}{2}}\tau_0. \quad (4.43)$$

Using this, we rewrite (4.42) in the form

$$\begin{aligned} H(\tau_0) = &-2(\pi)^{\frac{1}{2}} + (\pi/2)^{\frac{1}{2}} + 2(\pi)^{\frac{1}{2}}e^{-\tau_0^2/4} \\ &- (\pi)^{\frac{1}{2}}\tau_0\int_{\tau_0}^\infty d\mu e^{-\mu^2/4} - 2e^{-\tau_0^2/4}\int_{\tau_0}^\infty d\mu e^{-\mu^2/4} \\ &+ \tfrac{1}{2}\tau_0\left(\int_{\tau_0}^\infty d\mu e^{-\mu^2/4}\right)^2 + 2\int_{\tau_0}^\infty d\mu e^{-\mu^2/2} \\ &+ (2\pi)^{\frac{1}{2}}\tau_0\int_{\tau_0}^\infty d\mu e^{-\mu^2/2} - (\pi/2)^{\frac{1}{2}}e^{-\tau_0^2/2} \\ &- (\pi/2)^{\frac{1}{2}}\frac{d\xi_0}{d\tau_0} + \frac{d\xi_0}{d\tau_0}\int_{\tau_0}^\infty d\mu e^{-\mu^2/2} \\ &- \xi_0 e^{-\tau_0^2/2} - \frac{d}{d\tau_0}(\eta_1 + \eta_2). \end{aligned} \quad (4.44)$$

In order to satisfy the uniformity condition (4.21), we set

$$\eta_1 + \eta_2 = -(2 - (2)^{-\frac{1}{2}})(\pi)^{\frac{1}{2}}\tau_0. \quad (4.45)$$

Furthermore, in order to satisfy the differential uniformity condition, (4.22), we have to remove terms containing $e^{-\tau_0^2/4}$. We set

$$\frac{d\xi_0}{d\tau_0} = 2(2)^{\frac{1}{2}}e^{-\tau_0^2/4} - (2)^{\frac{1}{2}}\tau_0\int_{\tau_0}^\infty d\mu e^{-\mu^2/4}.$$

Integrating, we obtain

$$\begin{aligned} \xi_0 &= 2(2)^{\frac{1}{2}}\int_0^{\tau_0} d\lambda e^{-\mu^2/4} \\ &\quad - (2)^{\frac{1}{2}}\int_0^{\tau_0} d\lambda\lambda\int_\lambda^\infty d\mu e^{-\mu^2/4} \\ &= (2)^{\frac{1}{2}}\int_0^{\tau_0} d\lambda e^{-\lambda^2/4} \\ &\quad - (2)^{-\frac{1}{2}}\tau_0^2\int_{\tau_0}^\infty d\mu e^{-\mu^2/4} + (2)^{\frac{1}{2}}\tau_0 e^{-\tau_0^2/4}, \end{aligned}$$

or, rearranging slightly,

$$\begin{aligned} \xi_0 = (2\pi)^{\frac{1}{2}} - (2)^{\frac{1}{2}}\int_{\tau_0}^\infty d\lambda e^{-\lambda^2/4} + (2)^{\frac{1}{2}}\tau_0 e^{-\tau_0^2/4} \\ - \frac{\tau_0^2}{(2)^{\frac{1}{2}}}\int_{\tau_0}^\infty d\mu e^{-\mu^2/4}. \end{aligned} \quad (4.46)$$

Substituting (4.45) and (4.46) into (4.44), we have

$$\begin{aligned} H(\tau_0) = &\tfrac{1}{2}\tau_0\left(\int_{\tau_0}^\infty d\mu e^{-\mu^2/4}\right)^2 + 2\int_{\tau_0}^\infty d\mu e^{-\mu^2/2} \\ &+ (2\pi)^{\frac{1}{2}}\tau_0\int_{\tau_0}^\infty d\mu e^{-\mu^2/2} - (\pi/2)^{\frac{1}{2}}e^{-\tau_0^2/2} \\ &+ \left(2(2)^{\frac{1}{2}}e^{-\tau_0^2/4} - (2)^{\frac{1}{2}}\tau_0\int_{\tau_0}^\infty d\mu e^{-\mu^2/4}\right) \\ &\times\int_{\tau_0}^\infty d\mu e^{-\mu^2/2} - (2\pi)^{\frac{1}{2}}e^{-\tau_0^2/2} \\ &+ (2)^{\frac{1}{2}}e^{-\tau_0^2/2}\int_{\tau_0}^\infty d\mu e^{-\mu^2/4} - (2)^{\frac{1}{2}}\tau_0 e^{-3\tau_0^2/4} \\ &+ (2)^{-\frac{1}{2}}\tau_0^2 e^{-\tau_0^2/2}\int_{\tau_0}^\infty d\mu e^{-\mu^2/4}. \end{aligned} \quad (4.47)$$

Thus, we have

$$F^{(2)}(\tau_0) = \int_0^{\tau_0} d\mu H(\mu), \quad (4.48)$$

$$F^{(1)}(\tau_0) = 1 - e^{-\tau_0^2/2} + \tau_0\int_{\tau_0}^\infty d\mu e^{-\mu^2/2}, \quad (4.49)$$

$$\begin{aligned} f^{(0)}(\tau_0) &= \exp\{\epsilon\xi_1 + \epsilon^2(\eta_1 + \eta_2)\} \\ &= \exp\{-\epsilon(\pi/2)^{\frac{1}{2}}\tau_0 - \epsilon^2(2 - (2)^{-\frac{1}{2}}(\pi)^{\frac{1}{2}}\tau_0)\}. \end{aligned} \quad (4.50)$$

The relation between τ_0 and t is given by

$$\begin{aligned} t = \tau_0 + \epsilon\Big(&2(\pi)^{\frac{1}{2}} - (2)^{\frac{1}{2}}\int_{\tau_0}^\infty d\lambda e^{-\lambda^2/4} + (2)^{\frac{1}{2}}\tau_0 e^{-\tau_0^2/4} \\ &- \tau_0^2\int_{\tau_0}^\infty d\mu e^{-\tau_0^2/4}\Big) + O(\epsilon^2), \end{aligned} \quad (4.51)$$

or, inverting,

$$\begin{aligned} \tau_0 = t - \epsilon\Big(&2(\pi)^{\frac{1}{2}} - (2)^{\frac{1}{2}}\int_t^\infty d\mu e^{-\mu^2/4} + (2)^{\frac{1}{2}}te^{-t^2/4} \\ &- (2)^{-\frac{1}{2}}t^2\int_t^\infty d\mu e^{-\mu^2/4}\Big) + O(\epsilon^2). \end{aligned} \quad (4.52)$$

For large t, these expressions can be simplified as follows:

$$\tau_0 \sim t - \epsilon 2(\pi)^{\frac{1}{2}} + O(e^{-t^2/2}/t^5), \quad (4.53)$$

$$H \sim -(\pi/2)^{\frac{1}{2}}e^{-t^2/2}, \quad (4.54)$$

$$F^{(2)} \sim C - (\pi/2)^{\frac{1}{2}}e^{-t^2/2}/t, \quad C = \int_0^\infty dt H(t), \quad (4.55)$$

$$F^{(1)} \sim 1 - 2(e^{-t^2/2}/t^3); \quad (4.56)$$

$$^{(0)} \sim e^{-t\sqrt{\epsilon}}(-(2)^{-\frac{1}{2}}\epsilon - (2 - (2)^{-\frac{1}{2}})\epsilon^2)\{1 - \epsilon^2(2)^{\frac{1}{2}}\pi\}. \quad (4.57)$$

Thus, the dominant behavior of f for long times is

$$\begin{aligned} f = (A_0 + \epsilon A_1 + \epsilon^2 A_2)e^{-\epsilon\gamma_1 t - \epsilon^2\gamma_2 t} \\ + \left(\epsilon\frac{B_0}{t} + \frac{\epsilon^2 B_1}{t^3}\right)e^{-t^2/2 - \epsilon\gamma_1 t - \epsilon^2\gamma_2 t}. \end{aligned} \quad (4.58)$$

Here again we notice that there are two parts to the solution, namely, a finite slowly varying part and a small quickly varying part which decays away very quickly as a Gaussian.

5. CONCLUDING REMARKS

In the foregoing examples we have indicated a way of utilizing the freedom available from extension towards removing the nonuniformities of perturbation theory. By this method we have been able to obtain not only the leading behavior of f, but the higher-order corrections as well. Knowing the behavior of f, it is an easy matter to obtain g for this model in terms of a quadrature

$$\tilde{g} = i\mathbf{k}\cdot\mathbf{w}\tilde{U}\int_0^t dz e^{-i\mathbf{k}\cdot\mathbf{v}(t-z)}f(z).$$

In the first part of the paper we showed that this model has features analogous to kinetic theory. The synchronization method of Bogoliubov and the simple time scales method failed to give convergent higher-order corrections. We showed that this should be attributed to a nonuniform ordering of g. We got around this difficulty by two different methods: the first by reordering g, and the other by converting the pair of equations into one integrodifferential equation and then extending the time variable.

The method outlined in this paper could have wide application. Several problems in physics reduce to an equation of the form (4.1)—pair correlation in a plasma, linearized Vlasov equation, Wigner–Weisskopf model for radioactive decay, to mention a few. Furthermore, the technique presented here is not restricted to linear problems or to problems where the integral is a convolution.

Note added in proof: We have established recently [to be published in the *Proceedings of the Symposium on Kinetic Theory*, R. Liboff, Ed. (Cornell University, June 1969)] that the model equations (2.1) and (2.2) correspond to special spherical harmonics of a Lorentz gas.

APPENDIX A: REORDERING IN KINETIC THEORY

Following the line of reasoning presented in Sec. 3, we now derive the Fokker–Planck equation for a spatially uniform system of particles interacting through a weak spherically symmetric potential.[1,2,3] For the purposes of ordering, it is convenient to nondimensionalize all the quantities by setting $f = F/V^3$, $g = G/V^6$, $\mathbf{x} = r_0\boldsymbol{\xi}$, $\mathbf{v} = V\mathbf{u}$, $t = \tau(r_0/V)$, and $\phi = \epsilon\Phi mV^2$. f is the one-particle distribution, g the pair correlation, V some average velocity, r_0 the range of the potential (assumed to be finite), ϕ the potential, and m the mass of each particle. The parameter ϵ is a measure of the strength of the potential. The weak-coupling limit corresponds to ϵ small and $nr_0^3 \sim 1$ (n is the number density).

After Fourier transforming, the first two equations of the hierarchy take the following form:

$$\frac{\partial F}{\partial \tau} = \epsilon n r_0^3 \int\int d^3k\, d^3u_2 \Phi(\mathbf{k})\left(-i\mathbf{k}\cdot\frac{\partial}{\partial \mathbf{u}_1}\right) G(\mathbf{k}, \mathbf{u}_1, \mathbf{u}_2), \tag{A1}$$

$$\frac{\partial G}{\partial \tau} + i\mathbf{k}\cdot(\mathbf{u}_1 - \mathbf{u}_2)G = \epsilon\Phi(\mathbf{k})i\mathbf{k}\cdot\left(\frac{\partial}{\partial \mathbf{u}_1} - \frac{\partial}{\partial \mathbf{u}_2}\right)F(\mathbf{u}_1)F(\mathbf{u}_2) + O(\epsilon^2). \tag{A2}$$

We shall consider a simple initial value problem, i.e., $G(\tau = 0) = 0$.

If we assume that the right side of (A2) will always remain $O(\epsilon)$, it is clear that for finite times, $G \sim \epsilon$, so that $\partial F/\partial\tau \sim \epsilon^2$. The adiabatic assumption corresponds to saying the following. Since $\partial F/\partial\tau \sim \epsilon^2$, we could consider F as remaining stationary in the second equation for finite times, and also that for long times ($t \sim \epsilon^{-2}$)G will depend on τ only through F. The difficulty with this assumption is that it does not hold uniformly for all values of k. (There is another nonuniformity when $\mathbf{u}_1 - \mathbf{u}_2 = 0$. For our purposes it is sufficient to assume absence of such "parallel motion." For more details the reader is referred to Ref. 3.) It is indeed correct for finite k, but a simple calculation shows that the contribution to the collision integral comes from small values of k. In fact, the asymptotic solution for G, using Bogoliubov's assumption, is[1]

$$G \sim \epsilon\Phi(\mathbf{k})\mathbf{k}\cdot\left(\frac{\partial}{\partial \mathbf{u}_1} - \frac{\partial}{\partial \mathbf{u}_2}\right)F(\mathbf{u}_1)F(\mathbf{u}_2) \times\left[\frac{P}{\mathbf{k}\cdot(\mathbf{u}_1 - \mathbf{u}_2)} + \pi i\delta(\mathbf{k}\cdot\mathbf{u}_1 - \mathbf{k}\cdot\mathbf{u}_2)\right].$$

For a spherically symmetric potential, the principal part integrates to zero in the collision integral and only the δ function contributes. Considering the facts that the solution thus obtained for G is singular at $\mathbf{k}\cdot(\mathbf{u}_1 - \mathbf{u}_2) = 0$ and that the contribution to the collision integral comes from the neighborhood of $k_\parallel = 0$ [$k_\parallel$ stands for the component along $(\mathbf{u}_1 - \mathbf{u}_2)$], one should look at the equations more closely for small values of $k_\parallel$ and large values of τ. For this purpose, we reorder the terms in the two equations by setting $\tau = \tau'/\epsilon^2$, $k_\parallel = \epsilon^2 k_\parallel'$, and $G = (1/\epsilon)G'$. Then

we have

$$\frac{\partial F}{\partial \tau'} = nr_0^3 \iiint d^2k_\perp \, dk'_\parallel \, d^3u_2 \Phi(\mathbf{k}_\perp) \times \left(-i\mathbf{k}_\perp \cdot \frac{\partial}{\partial \mathbf{u}_1}\right) G' + O(\epsilon^2), \quad \text{(A3)}$$

$$\frac{\partial G'}{\partial \tau'} + ik'_\parallel \, |\mathbf{u}_1 - \mathbf{u}_2| \, G' = \Phi(\mathbf{k}_\perp) i\mathbf{k}_\perp \cdot \left(\frac{\partial}{\partial \mathbf{u}_1} - \frac{\partial}{\partial \mathbf{u}_2}\right) F(\mathbf{u}_1) F(\mathbf{u}_2) + O(\epsilon^2). \quad \text{(A4)}$$

Now the two equations are coupled, and G' and F evolve on the same time scale. Here we see explicitly the breakdown of the adiabatic assumption in the very regime which is relevant for the collision integral. As it turns out, although the kinetic equation obtained by solving (A4) and substituting into (A3) will be the same as that obtained by using the adiabatic assumption, the correlation functions in the two cases will be different. The one obtained by reordering will be neither adiabatic nor singular.

Neglecting terms of the order ϵ^2, Eq. (A4) can be solved to obtain

$$G' = \Phi(\mathbf{k}_\perp) i\mathbf{k}_\perp \cdot \left(\frac{\partial}{\partial \mathbf{u}_1} - \frac{\partial}{\partial \mathbf{u}_2}\right) \times \int_0^{\tau'} d\lambda e^{-ik'_\parallel |\mathbf{u}_1 - \mathbf{u}_2| \lambda} F(\mathbf{u}_1, \tau' - \lambda) F(\mathbf{u}_2, \tau' - \lambda). \quad \text{(A5)}$$

Substituting this result into the right side of (A3), we obtain

$$\begin{aligned}\frac{\partial F}{\partial \tau'} &= (nr_0^3) \frac{\partial}{\partial \mathbf{u}_1} \cdot \int d^3u_2 \int d^2k_\perp \mathbf{k}_\perp \Phi^2(k_\perp) \mathbf{k}_\perp \cdot \left(\frac{\partial}{\partial \mathbf{u}_1} - \frac{\partial}{\partial \mathbf{u}_2}\right) \\ &\quad \times \int_0^{\tau'} d\lambda F(\mathbf{u}_1, t - \lambda) F(\mathbf{u}_2, t - \lambda) \\ &\quad \times \int_{-\infty}^{\infty} dk_\parallel e^{-ik_\parallel |\mathbf{u}_1 - \mathbf{u}_2| \lambda} \\ &= (nr_0^3) \frac{\partial}{\partial \mathbf{u}_1} \cdot \int d^3u_2 \int d^2k_\perp \mathbf{k}_\perp \Phi^2(\mathbf{k}_\perp) \mathbf{k}_\perp \cdot \left(\frac{\partial}{\partial \mathbf{u}_1} - \frac{\partial}{\partial \mathbf{u}_2}\right) \\ &\quad \times \frac{F(\mathbf{u}_1, t) F(\mathbf{u}_2, t)}{|\mathbf{u}_1 - \mathbf{u}_2|}.\end{aligned}$$

Since

$$\mathbf{k}_\perp \cdot \left(\frac{\partial}{\partial \mathbf{u}_1} - \frac{\partial}{\partial \mathbf{u}_2}\right) |\mathbf{u}_1 - \mathbf{u}_2| = 0,$$

this can be written in the well-known form

$$\frac{\partial F}{\partial \tau'} = (nr_0^3) \frac{\partial}{\partial \mathbf{u}_1} \cdot \iint d^3u_2 \, d^3k \delta(\mathbf{k} \cdot \mathbf{u}_1 - \mathbf{k} \cdot \mathbf{u}_2) \Phi^2(\mathbf{k}) \mathbf{k} \times \mathbf{k} \cdot \left(\frac{\partial}{\partial \mathbf{u}_1} - \frac{\partial}{\partial \mathbf{u}_2}\right) F(\mathbf{u}_1) F(\mathbf{u}_2). \quad \text{(A6)}$$

APPENDIX B: ASYMPTOTIC EXPANSION OF AN INTEGRAL

We present here an example where the stretching method can be used for the asymptotic evaluation of integrals. We consider the following integral which occurs in the statistical mechanics of plasmas:

$$I = \int_0^\infty dx e^{-x - \epsilon/x}, \quad \text{(B1)}$$

where ϵ is a small positive parameter. An expansion of I in powers of ϵ breaks down in the first order.

Let us now write

$$x = s + \epsilon\xi(s) + \cdots, \quad \text{(B2)}$$

where s is a new variable and ξ is, as yet, an undetermined function of s. We note that the singular behavior of the integrand occurs for small values of x. We assume that as $x \to \infty$, $s \to \infty$. Writing I in terms of s in powers of ϵ,

$$I = \int_z^\infty ds e^{-s} \left(1 - \frac{\epsilon}{s} - \epsilon\xi + \epsilon \frac{d\xi}{ds}\right) + O(\epsilon^2), \quad \text{(B3)}$$

where $x = 0$ when $s = z$. Rewriting, we obtain

$$I = e^{-z} + \epsilon \int_z^\infty ds \left(\frac{d\xi}{ds} - \xi - \frac{1}{s}\right) + O(\epsilon^2).$$

In order to keep the first-order term bounded, we are free to choose

$$\frac{d\xi}{ds} - \xi = \frac{1}{s}, \quad \text{(B4)}$$

with

$$\xi(\infty) = 0. \quad \text{(B5)}$$

Solving (B4), we obtain

$$\xi = -e^s \int_s^\infty dy \frac{e^{-y}}{y}. \quad \text{(B6)}$$

Thus, we have

$$I = e^z, \quad \text{(B7)}$$

where

$$z = \epsilon e^z \int_z^\infty dy \frac{e^{-y}}{y}. \quad \text{(B8)}$$

If z were finite or large, the right-hand side of (B8) would be small. Therefore, in order to satisfy (B8), z will have to be small. The leading behavior of z is then given by

$$z \sim \epsilon \log \epsilon \quad \text{(B9)}$$

and

$$I \sim 1 + \epsilon \log \epsilon. \quad \text{(B10)}$$

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Properties of Overcomplete and Nonorthogonal Basis Vectors*

D. J. Rowe†
Department of Physics and Astronomy, University of Rochester, Rochester, New York

(Received 25 June 1968)

An alternative to the Schmidt procedure is presented for the orthogonalization of a set of functions or state vectors. The method is particularly simple and ideally suited to the eigenvalue problem in a space spanned by nonorthonormal, and even overcomplete, basis vectors. The method is applied to the solution of the equation of motion with a non-unit-metric matrix and to the problem of eliminating spurious (or any other) states from a given vector space.

1. INTRODUCTION

There are several reasons why it may be desirable to work with a space spanned by nonorthogonal and perhaps overcomplete basis vectors. For example, one might wish to exploit competing groups or opposing coupling schemes, which separately diagonalize major components of the Hamiltonian. Thus one could attempt intermediate coupling calculations by mixing the lowest L–S with the lowest j–j coupled configurations; or it might be convenient to consider the competition of "pairing" versus "quadrupole" forces by mixing states classified by seniority with those of the SU_3 group.[1]

Again it is known that states of intermediate coupling can be extracted, with considerable accuracy, by angular-momentum projection from a deformed determinant. To improve such wavefunctions it has been suggested that one diagonalize the Hamiltonian in a space of states projected from different determinants.[2] Whether the original determinants were orthogonal or not, the projected states, in general, are not orthogonal. Analogous situations, which involve overcompleteness, also arise when states of a larger space are projected onto a smaller model space.

The problem, which actually stimulated this study, was to find a measure for the norm and a criterion for orthogonality of operators. The problem occurs, for example, in the equations-of-motion approach to spectroscopy,[3] when one seeks excited eigenstate creation operators, in terms of a set of basis operators. For this problem, it transpires that the appropriate combination rule for the scalar product of two operators $\Gamma_1^\dagger$ and $\Gamma_2^\dagger$ is

$$(\Gamma_1^\dagger, \Gamma_2^\dagger) \equiv \langle\varphi|\,[\Gamma_1, \Gamma_2^\dagger]\,|\varphi\rangle, \tag{1}$$

where φ is a suitable specified wavefunction.[4] In solving the equations of motion for excitation operators, one again, in general, encounters the problems of a nonorthonormal, and perhaps overcomplete, basis set.

In the following section we present the heart of this paper, which is an orthogonalization procedure. It is an alternative to the Schmidt procedure[5] which, for more than a few vectors, is very messy. The procedure is simply to diagonalize the metric matrix by a *unitary* transformation. Thus it necessitates only a standard diagonalization routine, which must be available anyway for an eigenvalue problem, even for an orthonormal basis.

The method is extremely simple, but although it is surely familiar to some persons, it does not appear to be widely appreciated. The perturbation limit of this method was in fact suggested many years ago by Löwdin.[6] The perturbation procedure is very useful if the basis vectors are already almost orthogonal but actually diverges if they are overcomplete.

In Sec. 3, the method is applied to the solution of the standard eigenvalue problem in Hilbert space and to the equations-of-motion problem in operator space.

It is shown in Sec. 4 that the technique also has other applications: in particular, to extract a spurious state, or any other state, from a given vector space.

2. ORTHOGONALIZATION PROCEDURE

Consider an arbitrary set of basis vectors $|\alpha_i\rangle$. If this set were orthonormal, the metric matrix N, whose elements are defined as the overlaps

$$N_{ij} = \langle\alpha_i\,|\,\alpha_j\rangle, \tag{2}$$

would be the unit matrix. But for a nonorthogonal set, N is not diagonal.

* Work supported in part by the U.S. Atomic Energy Commission.
† Present address: Department of Physics, University of Toronto.
[1] M. Harvey, private communication, 1968.
[2] I. Kelson, Phys. Letters **16**, 143 (1965); private communication, 1968.
[3] D. J. Rowe, Rev. Mod. Phys. **40**, 153 (1968).
[4] A different definition of the scalar product of two operators, appropriate for measuring group-symmetry breaking, has been given by J. B. French, Phys. Letters **26B**, 75 (1967).
[5] See, for example, P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Co., New York, 1953), p. 928.
[6] P.-O. Löwdin, J. Chem. Phys. **18**, 365 (1950).

From inspection of N it is apparent that it is a Hermitian matrix and can therefore be diagonalized by a unitary transformation

$$\Lambda = S^\dagger N S, \qquad S^\dagger S = I. \tag{3}$$

Now the elements of

$$\Lambda_{kl} = \lambda_k \delta_{kl} = \sum_{ij} S^*_{ik} \langle \alpha_i \,|\, \alpha_j \rangle S_{jl} \tag{4}$$

can be regarded as the overlaps of new basis vectors

$$\Lambda_{kl} = \langle \beta_k \,|\, \beta_l \rangle = \lambda_k \delta_{kl}, \tag{5}$$

given by the unitary transformation

$$|\beta_l\rangle = \sum_j S_{jl} |\alpha_j\rangle. \tag{6}$$

Thus the eigenvectors of the metric matrix form an orthogonal set with norms given by the eigenvalues.

Since all the new vectors are orthogonal, it follows that some eigenvalues must vanish if the original set were overcomplete. It is, therefore, a simple matter to eliminate the vectors of vanishing norm, to leave a linearly independent set. This set can then be made orthonormal by the further nonunitary but trivial transformation

$$|\bar{\beta}_l\rangle = (\lambda_l)^{-\frac{1}{2}} |\beta_l\rangle = (\lambda_l)^{-\frac{1}{2}} \sum_j S_{jl} |\alpha_j\rangle \tag{7}$$

to give the renormalized metric matrix

$$\bar{\Lambda} = I. \tag{8}$$

As an example, consider the overcomplete set

$$|\alpha_1\rangle = (5)^{-\frac{1}{2}} 5\hat{x},$$
$$|\alpha_2\rangle = (5)^{-\frac{1}{2}} (4\hat{x} + 3\hat{y}),$$
$$|\alpha_3\rangle = (5)^{-\frac{1}{2}} 5\hat{y},$$

where $\hat{x}$, $\hat{y}$ are orthogonal unit vectors. These vectors have the metric matrix

$$N = \begin{pmatrix} 5 & 4 & 0 \\ 4 & 5 & 3 \\ 0 & 3 & 5 \end{pmatrix},$$

which is diagonalized by a unitary transformation to give the eigenvalues and eigenvectors

$$\lambda_1 = 0, \quad |\beta_1\rangle = (50)^{-\frac{1}{2}} (4\,|\alpha_1\rangle - 5\,|\alpha_2\rangle + 3\,|\alpha_3\rangle) \equiv 0,$$
$$\lambda_2 = 5, \quad |\beta_2\rangle = (5)^{-1} (-3\,|\alpha_1\rangle + 4\,|\alpha_3\rangle) = (5)^{-\frac{1}{2}} (-3\hat{x} + 4\hat{y}),$$
$$\lambda_3 = 10, \quad |\beta_3\rangle = (50)^{-\frac{1}{2}} (4\,|\alpha_1\rangle + 5\,|\alpha_2\rangle + 3\,|\alpha_3\rangle) = (\tfrac{2}{5})^{\frac{1}{2}} (4\hat{x} + 3\hat{y}).$$

For the equations-of-motion problem in which an excitation operator is sought within a space spanned by a set of basis operators $\eta^\dagger_\alpha$, η_α, the metric matrix N is defined, according to (1), by the elements

$$N_{ij} = \langle \varphi | \, [\Gamma_i, \Gamma^\dagger_j] \, | \varphi \rangle, \tag{9}$$

where $\Gamma^\dagger_j$ runs over the set $\eta^\dagger_\alpha$, $-\eta_\alpha$. Thus N is the super matrix

$$N = \begin{pmatrix} U & V \\ -V^* & -U^* \end{pmatrix}, \tag{10}$$

where the submatrices are defined as

$$U_{\alpha\beta} = \langle \varphi | \, [\eta_\alpha, \eta^\dagger_\beta] \, | \varphi \rangle,$$
$$V_{\alpha\beta} = \langle \varphi | \, [\eta_\alpha, -\eta_\beta] \, | \varphi \rangle. \tag{11}$$

The only essential difference between this metric matrix and the more familiar one defined by (2) is that it is not positive-definite. In fact, it has vanishing trace. But U is Hermitian and V is antisymmetric so that N is once again Hermitian and can be diagonalized by a unitary transformation S [Eq. (3)].

The new set of operators $\zeta^\dagger_l$ defined by the transformation

$$\zeta^\dagger_l = \sum_j S_{jl} \Gamma^\dagger_j \tag{12}$$

now form an orthogonal set, according to the scalar product (1), which can be renormalized to give orthogonality relations

$$(\zeta^\dagger_k, \zeta^\dagger_l) \equiv \langle \varphi | \, [\zeta_k, \zeta^\dagger_l] \, | \varphi \rangle = \pm \delta_{kl} \tag{13}$$

and a renormalized metric matrix

$$\bar{\Lambda} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \tag{14}$$

3. APPLICATION TO EIGENVALUE PROBLEMS

Within the space spanned by a set of nonorthonormal basis vectors $|\alpha_i\rangle$, an eigenvector $|\lambda\rangle$ of a Hamiltonian H can be expanded as

$$|\lambda\rangle = \sum_i X_i(\lambda) |\alpha_i\rangle. \tag{15}$$

Its expansion coefficients are solutions of the secular equation

$$\sum_j \langle \alpha_i | \, H \, | \alpha_j \rangle \, X_j(\lambda) = E_\lambda \sum_j \langle \alpha_i \,|\, \alpha_j \rangle X_j(\lambda), \quad \text{for all } i, \tag{16}$$

which can be written in matrix form

$$HX(\lambda) = E_\lambda N X(\lambda), \tag{17}$$

with obvious notation.

One method of solving this equation is to seek values of E_λ for which the determinant $|H - E_\lambda N|$

vanishes. This method is no good, however, if the vector space is overcomplete, since the determinants $|H|$ and $|N|$ will vanish separately.

In any case, it is generally preferable to transform to an orthonormal basis, in order that standard matrix diagonalization routines can be employed.

Introducing first the unitary transformation S, which diagonalizes N, Eq. (17) becomes

$$(S^\dagger HS)[S^\dagger X(\lambda)] = E_\lambda \Lambda [S^\dagger X(\lambda)]. \tag{18}$$

If the vector space is overcomplete and Λ has a vanishing diagonal element, it is now a trivial matter to truncate the vector space, and hence the matrix equation (18), in order to eliminate the spurious vector of vanishing norm. We can, therefore, assume without any loss of generality that Λ has no vanishing diagonal elements. Making the further nonunitary, but trivial, transformation (7), we now obtain an eigenvalue equation of standard form

$$\mathcal{H}\mathcal{X}(\lambda) = E_\lambda \mathcal{X}(\lambda), \tag{19}$$

where

$$\mathcal{X}(\lambda) = \Lambda^{\frac{1}{2}} S^\dagger X(\lambda),$$
$$\mathcal{H} = \Lambda^{-\frac{1}{2}} S^\dagger H S \Lambda^{-\frac{1}{2}}. \tag{20}$$

In the equations of motion,[3] an excited eigenstate creation operator $O_\lambda^\dagger$ is expanded as

$$O_\lambda^\dagger = \sum_\alpha \{Y_\alpha(\lambda)\eta_\alpha^\dagger - Z_\alpha(\lambda)\eta_\alpha\} \tag{21}$$

and its expansion coefficients are determined from the equations of motion

$$\langle\varphi|\,[\delta O_\lambda, H, O_\lambda^\dagger]\,|\varphi\rangle = \omega_\lambda \langle\varphi|\,[\delta O_\lambda, O_\lambda^\dagger]\,|\varphi\rangle, \tag{22}$$

where ω_λ is the excitation energy $E_\lambda - E_0$, $|\varphi\rangle$ is the ground state, or some appróximation to it, and the double commutation is defined

$$2[\delta O_\lambda, H, O_\lambda^\dagger] \equiv [\delta O_\lambda, [H, O_\lambda^\dagger]] + [[\delta O_\lambda, H], O_\lambda^\dagger]. \tag{23}$$

Expansion of (22) gives a secular matrix equation of the form[3]

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} Y(\lambda) \\ Z(\lambda) \end{pmatrix} = \omega_\lambda \begin{pmatrix} U & V \\ -V^* & -U^* \end{pmatrix}\begin{pmatrix} Y(\lambda) \\ Z(\lambda) \end{pmatrix}, \tag{24}$$

which is reduced to standard RPA (random-phase-approximation) form

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B}^* & \mathcal{A}^* \end{pmatrix}\begin{pmatrix} \mathcal{Y}(\lambda) \\ \mathcal{Z}(\lambda) \end{pmatrix} = \omega_\lambda \begin{pmatrix} \mathcal{Y}(\lambda) \\ -\mathcal{Z}(\lambda) \end{pmatrix} \tag{25}$$

by the transformation

$$\begin{pmatrix} \mathcal{Y}(\lambda) \\ \mathcal{Z}(\lambda) \end{pmatrix} = \begin{pmatrix} \Omega^{\frac{1}{2}} & 0 \\ 0 & \Omega^{\frac{1}{2}} \end{pmatrix} S^\dagger \begin{pmatrix} Y(\lambda) \\ Z(\lambda) \end{pmatrix}, \tag{26}$$

where Ω is the diagonal positive-definite matrix defined by

$$\Lambda = \begin{pmatrix} \Omega & 0 \\ 0 & -\Omega \end{pmatrix}, \tag{27}$$

which we assume has no vanishing diagonal elements in order that $\Omega^{\frac{1}{2}}$ has an inverse. If it does have vanishing diagonal elements then the matrix equation can be truncated at the stage analogous to (18) to eliminate them.

4. ELIMINATION OF A GIVEN VECTOR FROM A SPACE

Suppose we have a space spanned, for simplicity, by n orthonormal basis vectors $|\alpha_i\rangle$, and that we wish to eliminate a given vector $|\gamma\rangle$ from this space.

The problem arises, for example, in the nuclear shell model, when one wishes to eliminate the spurious center-of-mass state from a given shell-model space before diagonalizing the Hamiltonian.[7]

The objective is achieved by adding $|\gamma\rangle$ to the set $|\alpha_i\rangle$ to form an overcomplete $(n+1)$-dimensional space, constructing the metric matrix which will have the form

$$N = \left(\begin{array}{c|ccccc} 1 & x & x & \cdots & x \\ \hline x & 1 & & & 0 \\ x & & 1 & & \\ \cdot & & & \cdot & \\ \cdot & & & & \cdot \\ \cdot & & & & \\ x & 0 & & & 1 \end{array}\right), \tag{28}$$

and diagonalizing it by a unitary transformation. The diagonalized metric matrix Λ should then be

$$\Lambda = S^\dagger N S = \begin{pmatrix} 0 & & & & & \\ & 2 & & & & \\ & & 1 & & & 0 \\ & & & 1 & & \\ & & & & \cdot & \\ & & & & & \cdot \\ & & 0 & & & \\ & & & & & 1 \end{pmatrix} \tag{29}$$

The vector of norm 2 is simply $\sqrt{2}\,|\gamma\rangle$ which, together with the vector of vanishing norm, can be removed to leave a set of $n-1$ orthonormal vectors all orthogonal to γ.

[7] E. Baranger and C. W. Lee, Nucl. Phys. **22**, 157 (1961).

To prove this, one simply notes that there exists a unitary transformation in the original n-dimensional space which makes one of the $|\alpha_i\rangle$ equal to $|\gamma\rangle$. After making such a unitary transformation, the metric matrix in the $(n+1)$-dimensional space would then become

$$N' = \begin{pmatrix} 1 & 1 & & & & \\ 1 & 1 & & & 0 & \\ & & 1 & & & 0 \\ & & & 1 & & \\ & 0 & & & \ddots & \\ & & & 0 & & 1 \end{pmatrix}, \tag{30}$$

which is trivially diagonalized to give (29).

Should there be a convergence problem in diagonalizing a matrix with almost all of its eigenvalues equal, the method is easily modified to avoid this difficulty. One simply multiplies all the basis vectors by different normalization factors, but $|\gamma\rangle$ must be given a normalization factor larger than any $|\alpha_i\rangle$. Then, upon diagonalization, the eigenvector with maximum norm is proportional to $|\gamma\rangle$ and can be removed together with the eigenvector of vanishing norm.

Note added in proof: Since submission of this paper it has been pointed out to the author that the orthogonalization procedure, described above, has been used by P. Goode and L. Zamick (preprint).

ACKNOWLEDGMENTS

The author wishes to thank Dr. J. B. French and Dr. D. S. Koltun for helpful discussion and suggestions.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Degenerate Representations of the Symplectic Groups II. The Noncompact Group $Sp(p, q)$

P. PAJAS
Nuclear Research Institute of the Czechoslovak Academy of Sciences
Řež, Czechoslovakia

(Received 4 April 1968)

Using a method based on geometrical properties of homogeneous spaces of rank one homeomorphic to coset spaces of Lie groups, a series of degenerate unitary irreducible representations of the noncompact symplectic group $Sp(p, q)$ is investigated. The representation spaces for a discrete series determined by two integer numbers and a continuous series determined by one real and one integer parameter are given, the corresponding basis functions being formed by the linear combinations of eigenfunctions of the Laplace–Beltrami operator of the considered space. Explicit formulas for the action of generators of $Sp(p, q)$ in these representations are obtained. The results provide a deeper insight into the structure of the two-parameter "not most degenerate" unitary representations.

1. INTRODUCTION

A number of physical problems ranging from an attempted relativistic extension of internal symmetries in particle physics, through the spectrum-generating noninvariance (or dynamical) groups for "classical" quantum-mechanical systems, to the labeling of states in nuclear shell theory are more or less responsible for interest in and a deeper knowledge of the properties of unitary irreducible representations of noncompact Lie groups. This is due to the possibility of organizing all physically interesting unitary representations of compact symmetry groups of a considered system into one irreducible unitary infinite-dimensional representation of a certain noncompact group. At the same time, the physical interest (as well as Nature's preference) is concentrated on the representations which leave the lowest possible number of invariants and operators to be physically interpreted. It is well known[1] that this property is guaranteed by the irreducible unitary representations (IUR) belonging to the so-called most degenerate series.

The restriction to the Lie groups means, in practice, restriction to the groups the compact real forms of which are $SO(2n)$, $SO(2n+1)$, $SU(n)$, and $Sp(n)$, i.e., the groups of transformations which preserve a

[1] I. M. Gel'fand and M. A. Naimark, Inst. Steklova **36**, 1 (1950).

To prove this, one simply notes that there exists a unitary transformation in the original n-dimensional space which makes one of the $|\alpha_i\rangle$ equal to $|\gamma\rangle$. After making such a unitary transformation, the metric matrix in the $(n+1)$-dimensional space would then become

$$N' = \begin{pmatrix} 1 & 1 & & & & \\ 1 & 1 & & & 0 & \\ & & 1 & & & 0 \\ & & & 1 & & \\ & 0 & & & \ddots & \\ & & & 0 & & 1 \end{pmatrix}, \tag{30}$$

which is trivially diagonalized to give (29).

Should there be a convergence problem in diagonalizing a matrix with almost all of its eigenvalues equal, the method is easily modified to avoid this difficulty. One simply multiplies all the basis vectors by different normalization factors, but $|\gamma\rangle$ must be given a normalization factor larger than any $|\alpha_i\rangle$. Then, upon diagonalization, the eigenvector with maximum norm is proportional to $|\gamma\rangle$ and can be removed together with the eigenvector of vanishing norm.

Note added in proof: Since submission of this paper it has been pointed out to the author that the orthogonalization procedure, described above, has been used by P. Goode and L. Zamick (preprint).

ACKNOWLEDGMENTS

The author wishes to thank Dr. J. B. French and Dr. D. S. Koltun for helpful discussion and suggestions.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Degenerate Representations of the Symplectic Groups II. The Noncompact Group $Sp(p, q)$

P. PAJAS
Nuclear Research Institute of the Czechoslovak Academy of Sciences
Řež, Czechoslovakia

(Received 4 April 1968)

Using a method based on geometrical properties of homogeneous spaces of rank one homeomorphic to coset spaces of Lie groups, a series of degenerate unitary irreducible representations of the noncompact symplectic group $Sp(p, q)$ is investigated. The representation spaces for a discrete series determined by two integer numbers and a continuous series determined by one real and one integer parameter are given, the corresponding basis functions being formed by the linear combinations of eigenfunctions of the Laplace–Beltrami operator of the considered space. Explicit formulas for the action of generators of $Sp(p, q)$ in these representations are obtained. The results provide a deeper insight into the structure of the two-parameter "not most degenerate" unitary representations.

1. INTRODUCTION

A number of physical problems ranging from an attempted relativistic extension of internal symmetries in particle physics, through the spectrum-generating noninvariance (or dynamical) groups for "classical" quantum-mechanical systems, to the labeling of states in nuclear shell theory are more or less responsible for interest in and a deeper knowledge of the properties of unitary irreducible representations of noncompact Lie groups. This is due to the possibility of organizing all physically interesting unitary representations of compact symmetry groups of a considered system into one irreducible unitary infinite-dimensional representation of a certain noncompact group. At the same time, the physical interest (as well as Nature's preference) is concentrated on the representations which leave the lowest possible number of invariants and operators to be physically interpreted. It is well known[1] that this property is guaranteed by the irreducible unitary representations (IUR) belonging to the so-called most degenerate series.

The restriction to the Lie groups means, in practice, restriction to the groups the compact real forms of which are $SO(2n)$, $SO(2n+1)$, $SU(n)$, and $Sp(n)$, i.e., the groups of transformations which preserve a

[1] I. M. Gel'fand and M. A. Naimark, Inst. Steklova **36**, 1 (1950).

symmetric bilinear form in even- and odd-dimensional real space ($\mathcal{R}_{2n}$ and $\mathcal{R}_{2n+1}$), in a complex space $\mathcal{C}_n$, and a space of quaternions Q_n, respectively. From the viewpoint of physical application we are interested not only in the representations of the groups themselves but, and sometimes especially, in the representations of the corresponding Lie algebras, the elements and invariants of which can have direct connection with physical quantities. Therefore, in the majority of papers[2] dealing with construction of IUR of these groups and their noncompact extensions the infinitesimal approach has been used. A method of constructing most degenerate representations of the noncompact orthogonal groups $SO(p, q)$ for arbitrary p and q, based on the geometrical properties of homogeneous spaces of rank one has been widely developed at the ICTP, Trieste,[3,4] and further generalized to unitary groups $U(p, q)$ and $SU(p, q)$ in Ref. 5. Finally, in Ref. 6 (which constitutes the first part of the present series of papers, hereafter referred to as Paper I) this method has been employed for construction of IUR of the compact symplectic group $Sp(n)$ using the generalization from complex to quaternionic variables. The main idea of the method is, in fact, reduced to the problem of finding appropriate eigenfunctions of the Laplace–Beltrami operator Δ of the space, which is homeomorphic to a homogeneous space

$$X = G/G_0, \tag{1.1}$$

G being the considered group and G_0 some closed subgroup of it.

In order to get the IUR of highest degeneration, it is necessary (according to the Gel'fand theorem[7]) to choose the space (1.1) of lowest possible rank (i.e., with the lowest possible number of invariants with respect to the action of G, defined on X). In the Trieste approach, these spaces have been chosen with G_0 in (1.1), generally speaking, noncompact when G is noncompact. This has enabled the most degenerate representations of the considered groups to be treated in a unique way on the spaces homeomorphic to the ordinary hyperboloidal hypersurfaces in a generalized Minkowski space of a definite dimension.

In this paper we shall investigate the properties of degenerate representations of the noncompact group $Sp(p, q)$ of unitary transformations in the $p + q$ quaternionic unitary space $Q^{p+q}_{p,q}$, which leaves invariant the quaternionic bilinear form

$$B(q, q') = \sum_{s=1}^{p+q} q_s \bar{q}'_s \epsilon_s, \tag{1.2}$$

where $q = (q_1, \cdots, q_p; q_{p+1}, \cdots, q_{p+q})$ is an element of $Q^{p+q}_{p,q}$, a $(p + q)$-dimensional quaternionic space with p $(+1)$'s and q (-1)'s on the matrix-tensor diagonal. Therefore, $\epsilon_s = +1$ for $s = 1, \cdots, p$ and -1 for $s = p + 1, \cdots, p + q$. An equivalent definition of $Sp(p, q)$ is related to unitary symplectic transformations of the $2(p + q)$-dimensional unitary complex space $C^{2(p+q)}_{2p,2q}$, where an antisymmetric exterior form

$$E(z, z') = \sum_{s=1}^{p+q} (z_s z'_{-s} - z_{-s} z'_s)\epsilon_s \tag{1.3}$$

is preserved together with the indefinite Hermitian form

$$H(z, z') = \sum_{s=1}^{p} (z_s z'^{*}_s + z_{-s} z'^{*}_{-s})\epsilon_s. \tag{1.4}$$

Here $z = (z_1, \cdots, z_p; z_{p+1}, \cdots, z_{p+q}; z_{-1}, \cdots, z_{-p}; z_{-p-1}, \cdots, z_{-p-q}) \in C^{2(p+q)}_{2p,2q}$ and the relation to the quaternionic coordinates is given by

$$q_s = z_s + j z_{-s}, \quad j^2 = -1, ji = -ij, i = (-1)^{\frac{1}{2}}.$$

Since we are mainly interested in the most degenerate representations, we are looking for a homogeneous space of rank one, or a space close to it by its properties on which the group acts transitively.

From Table I of Paper I we see that the appropriate choice is given by

$$X_1^{p,q} = Sp(p, q)/Sp(p - 1, q) \otimes Sp(1)$$

or

$$X_2^{p,q} = Sp(p, q)/Sp(p, q - 1) \otimes Sp(1), \tag{1.5}$$

which are the so-called quaternion hyperbolic spaces. Nevertheless, the spaces

$$X_+^{4p,4q} = Sp(p, q)/Sp(p - 1, q)$$

and

$$X_-^{4p,4q} = Sp(p, q)/Sp(p, q - 1) \tag{1.6}$$

are closely related to X_1 and X_2, respectively, and, moreover, simple models of them exist. So the space $X_+^{4p,4q}$ is homeomorphic to the unitary hyperboloid in the $(p + q)$-dimensional quaternionic space $Q^{p+q}_{p,q}$, where it is defined by the equation $B(q, q) = 1$,

[2] M. A. B. Bég and H. Ruegg, J. Math. Phys. **6**, 677 (1965); V. Bargmann, Ann. Math. **48**, 568 (1947); A. Kihlberg, Arkiv Fysik **30**, 121 (1965); J. Dixmier, Bull. Soc. Math. France **89**, 9 (1961); I. T. Todorov, ICTP Preprint IC/66/71, Trieste, 1966; G. E. Baird and L. C. Biedenharn, J. Math. Phys. **4**, 1449 (1963); H. Bacry, J. Nuyts, and L. Van Hove, Nuovo Cimento **35**, 510 (1965); R. L. Anderson, J. Fischer, and R. Rączka, Proc. Roy. Soc. (London) **302A**, 491 (1968).

[3] R. Rączka, N. Limić, and J. Niederle, J. Math. Phys. **7**, 1861 (1966); N. Limić, J. Niederle, and R. Rączka, *ibid.* **7**, 2026 (1966).

[4] N. Limić, J. Niederle, and R. Rączka, J. Math. Phys. **8**, 1109 (1967).

[5] R. Rączka and J. Fischer, Commun. Math. Phys. **3**, 233 (1966); J. Fischer and R. Rączka, *ibid.* **4**, 8 (1967).

[6] P. Pajas and R. Rączka, J. Math. Phys. **9**, 1188 (1968), Paper I of this series.

[7] I. M. Gel'fand, Am. Math. Soc. Transl. Ser. 2, **37**, 31 (1964).

while $X_-^{4p,4q}$ is homeomorphic to the hyperboloid defined by $B(q,q) = -1$.

According to the Helgason lemma,[8] the Laplace–Beltrami operator of the space of rank one generates the ring of invariant operators of the group G on the space. The group G which acts transitively on both $X_+^{4p,4q}$ and $X_-^{4p,4q}$ is the group $Sp(p,q) \otimes Sp(1)$.[9] Therefore, the eigenfunctions of the Laplace–Beltrami operator on $X_\pm^{4p,4q}$ corresponding to a definite eigenvalue of it should provide a basis for a representation space of the group $Sp(p,q) \otimes Sp(1)$, this being further reduced to subspaces irreducible with respect to the action of the group $Sp(p,q)$ alone.

Generally, the Laplace–Beltrami operator of X is defined as a second-order differential operator in coordinates on the space X by

$$\Delta(X) = (\bar{g})^{-\frac{1}{2}}\partial_\alpha g^{\alpha\beta}(X)(\bar{g})^{\frac{1}{2}}\partial_\beta, \tag{1.7}$$

where $g^{\alpha\beta}(X)$ is defined by

$$g^{\alpha\beta}(X)g_{\beta\gamma}(X) = \delta_\gamma^\alpha, \tag{1.8}$$

$g_{\alpha\beta}(X)$ being the matrix tensor of the space X and

$$\bar{g} = |\det\{g_{\alpha\beta}(X)\}|. \tag{1.9}$$

In Sec. 2 we give explicit expressions for the Laplace–Beltrami operators associated with the spaces $X_+^{4p,4q}$ and $X_-^{4p,4q}$ defined above, together with its eigenfunctions and spectra of eigenvalues. From the system of harmonic functions thus obtained, we form Hilbert spaces as representation spaces of the group $Sp(p,q) \otimes Sp(1)$; we study the properties of representation spaces of $Sp(p,q)$ in Sec. 3. The investigation is performed for the discrete and continuous parts of the spectrum of $\Delta(X)$, respectively.

2. HARMONIC FUNCTIONS ASSOCIATED WITH THE GROUP $Sp(p,q)$

In what follows we use only the complex variables to avoid complications with noncommutativity of the quaternionic algebra. The detailed discussion is made for the space $X_+^{4p,4q}$ only because other cases are simply related to it. First of all, let us introduce a convenient inner coordinate system on the hyperboloid (1.6). In order to obtain a possibility of direct decomposition of the irreducible representation spaces of $Sp(p,q)$ with respect to the maximal compact subgroup $Sp(p) \otimes Sp(q)$, we introduce the following parametrization of the coordinates z_i, z_{-i} $(i = 1, \cdots, p+q)$.

Let us suppose the coordinate systems on the compact subspaces of $X_+^{4p,4q}$ to be defined and let corresponding coordinates be denoted by a prime. Then we define

$$z_{\pm k} = z'_{\pm k}\cosh\omega \quad \text{for} \quad k = 1, \cdots, p \tag{2.1}$$

and

$$z_{\pm k} = z'_{\pm k}\sinh\omega \quad \text{for} \quad k = p+1, \cdots, p+q. \tag{2.2}$$

We recall from Paper I that the parametrization of z'_k and z'_{-k} is given for $k = 1, \cdots, p$ by

$$z'_{\pm k} = z''_{\pm k}\sin\xi_{s+1} \quad \text{for} \quad k = 1, \cdots, s < p, \tag{2.3}$$

while

$$z_{s+1} = \rho\exp\{i\varphi_{s+1}\}\cos\vartheta_{s+1}\cos\xi_{s+1} \tag{2.4}$$

and

$$z_{-s-1} = \rho\exp\{i\psi_{s+1}\}\sin\vartheta_{s+1}\cos\xi_{s+1}. \tag{2.5}$$

Starting from

$$z_1 = \rho\exp\{i\varphi_1\}\cos\vartheta_1 \tag{2.6}$$

and

$$z_{-1} = \rho\exp\{i\psi_1\}\sin\vartheta_1, \tag{2.7}$$

together with the similar parametrization for $k = p+1, \cdots, p+q$, one gets the parametrization of the whole $X_+^{4p,4q}$ space in a recursive way. To distinguish the two compact subspaces we introduce a tilde above the parameters corresponding to the subspace spanned by $z_{p+1}, \cdots, z_{p+q}$; $z_{-(p+1)}, \cdots, z_{-(p+q)}$ coordinates.

The regions of the $4(p+q)-1$ variables thus introduced are as follows:

$$\begin{aligned}
&\left.\begin{aligned}\varphi_k, \psi_k &\in [0, 2\pi)\\ \vartheta_k &\in [0, \pi/2]\end{aligned}\right\} && (k = 1, \cdots, p),\\
&\xi_k \in [0, \pi/l2] && (k = 2, \cdots, p),\\
&\left.\begin{aligned}\tilde{\varphi}_k, \tilde{\psi}_k &\in [0, 2\pi)\\ \tilde{\vartheta}_k &\in [0, \pi/l]\end{aligned}\right\} && (k = p+1, \cdots, p+q),\\
&\xi_k \in [0, \pi/2] && (k = p+2, \cdots, p+q),
\end{aligned} \tag{2.8}$$

and

$$\omega \in [0, \infty), \quad \rho = 1.$$

It follows that the space $X_+^{4p,4q}$ is covered by the coordinates (2.1)–(2.7) just once.

In the coordinates (2.8) the Laplace–Beltrami operator as defined by (1.6) acquires the form

$$\Delta(X_+^{4p,4q}) = \hat{L}(\omega) + \frac{\Delta(X^{4p-1})}{(\cosh\omega)^2} - \frac{\Delta(X^{4q-1})}{(\sinh\omega)^2}, \tag{2.9}$$

where $\Delta(X^{4p-1})$ and $\Delta(X^{4q-1})$, given explicitly in Paper I, are the Laplace–Beltrami operators of the compact subspaces X^{4p-1} and X^{4q-1} defined by the

[8] S. Helgason, *Differential Geometry and Symmetric Spaces* (Academic Press Inc., New York, 1962).

[9] C. Chevalley, *Theory of Lie Groups I* (Princeton University Press, Princeton, N.J., 1964); W. Hsien-Chung, Ann. Math. 55, 177 (1925).

equations

$$\sum_{s=1}^{p}(z_s z_s^* + z_{-s}z_{-s}^*) = \sum_{s=1}^{q}(z_{p+s}z_{p+s}^* + z_{-p-s}z_{-p-s}^*) = 1. \tag{2.10}$$

The operator $\hat{L}(\omega)$ is given by

$$\hat{L}(\omega) = -\frac{1}{(\cosh\omega)^{4p-1}(\sinh\omega)^{4q-1}} \times \frac{\partial}{\partial\omega}(\cosh\omega)^{4p-1}(\sinh\omega)^{4q-1}\frac{\partial}{\partial\omega}. \tag{2.11}$$

In our parametrization the eigenequation

$$(\Delta(X_+^{4p,4q}) - \lambda)V_\alpha^\lambda = 0 \tag{2.12}$$

is reduced to the set of ordinary differential equations if we assume the solution in the form

$$V_\alpha^\lambda(\omega, \sigma_p, \tilde{\sigma}_q) = \Omega_{L_p,\tilde{L}_q}^\lambda(\omega)Y^{L_p,\beta}(\sigma_p)Y^{\tilde{L}_q,\tilde{\beta}}(\tilde{\sigma}_q), \tag{2.13}$$

where the functions $Y^{L_s,\beta}(\sigma_s)$ are those obtained in Paper I, σ's standing for the set of variables $\{\xi_s, \xi_{s-1}, \cdots, \xi_2; \vartheta_s, \vartheta_{s-1}, \cdots, \vartheta_1; \varphi_s, \varphi_{s-1}, \cdots, \varphi_1; \psi_s, \psi_{s-1}, \cdots, \psi_1\}$ and the Greek label β denoting all the remaining indices necessary to distinguish the degenerate solutions.

The function $\Omega_{L_p,\tilde{L}_q}^\lambda(\omega)$, which is a solution of the equation

$$\left(\hat{L}(\omega) - \frac{L_p(L_p+4p-2)}{(\cosh\omega)^2} + \frac{\tilde{L}_q(\tilde{L}_q+4q-2)}{(\sinh\omega)^2} - \lambda\right) \times \Omega_{L_p,\tilde{L}_q}^\lambda(\omega) = 0, \tag{2.14}$$

regular in $\omega = 0$ and finite for $\omega \to \infty$, is given by

$$\Omega_{L_p,\tilde{L}_q}^\lambda(\omega) = N^{-\frac{1}{2}}(\tanh\omega)^{\tilde{L}_q}(\cosh\omega)^{a(\lambda)}{}_2F_1(\alpha,\beta;\gamma;\tanh^2\omega), \tag{2.15}$$

where

$$a(\lambda) = -(2p+2q-1) - [(2p+2q-1)^2 - \lambda]^{\frac{1}{2}}. \tag{2.16}$$

If we represent λ as

$$\lambda = -L(L+4p+4q-2), \tag{2.17}$$

we get

$$a(\lambda) = -L - 4p - 4q + 2,$$

while the parameters of the hypergeometrical function in (2.15) are

$$\alpha = \tfrac{1}{2}(L + L_p + \tilde{L}_q + 4p + 4q - 2),$$
$$\beta = \tfrac{1}{2}(L - L_p + \tilde{L}_q + 4q), \tag{2.18}$$

and

$$\gamma = \tilde{L}_q + 2q.$$

In the case when

$$\lambda < (2p+2q-1)^2, \tag{2.19}$$

we get the solutions square-integrable on $X_+^{4p,4q}$ for

$$\beta = -n, \quad n = 0, 1, \cdots. \tag{2.20}$$

From (2.19) and (2.20) follows a condition on the numbers L, L_p, and $\tilde{L}_q$:

$$L = L_p - \tilde{L}_q - 4q - 2n > -2p - 2q + 1, \quad n = 0, 1, \cdots. \tag{2.21}$$

The corresponding functions $V_{L_p,\tilde{L}_q,\beta,\tilde{\beta}}^L(\omega, \sigma_p, \tilde{\sigma}_q)$ form a discrete set of harmonic functions related to the group $Sp(p,q) \otimes Sp(1)$. The solution remains regular for

$$\lambda \geq (2p+2q-1)^2, \tag{2.22}$$

but then we have

$$L = -2p - 2q + 1 + i\Lambda, \tag{2.23}$$

where $\Lambda \geq 0$. The harmonic functions corresponding to the continuous part (2.23) of the spectrum of $\Delta(X_+^{p,q})$ are now

$$\Omega_{L_p,\tilde{L}_q}^\Lambda(\omega) = M^{-\frac{1}{2}}(\tanh\omega)^{\tilde{L}_q}(\cosh\omega)^{-2p-2q+1-i\Lambda} \times {}_2F_1\left(\frac{\tilde{L}_q + L_p + 2p + 2q - 1 - i\Lambda}{2}, \frac{\tilde{L}_q - L_p - 2p + 2q + 1 - i\Lambda}{2}; \gamma; \tanh^2\omega\right). \tag{2.24}$$

The normalization factor N in (2.15) is

$$N = \frac{[\Gamma(\tilde{L}_q+2q)]^2\Gamma(\frac{1}{2}(-L+L_p-\tilde{L}_q-4q+2))\Gamma(\frac{1}{2}(L+L_p-\tilde{L}_q+4p))}{2(L+2p+2q-1)\Gamma(\frac{1}{2}(-L+L_p+\tilde{L}_q))\Gamma(\frac{1}{2}(L+L_p+\tilde{L}_q+4p+4q-2))}, \tag{2.25}$$

while for the factor M in (2.24), which corresponds to the normalization of $\Omega_{L_p,\tilde{L}_q}^\Lambda$ to the delta function $\delta(\Lambda - \Lambda')$, the expression

$$M = \frac{2\pi|\Gamma(i\Lambda)|^2\,|\Gamma(\tilde{L}_q+2q)|^2}{|\Gamma(\frac{1}{2}(\tilde{L}_q+L_p+2p+2q-1+i\Lambda))|^2\,|\Gamma(\frac{1}{2}(\tilde{L}_q-L_p-2p+2q+1+i\Lambda))|^2} \tag{2.26}$$

has been found.[4]

The left-invariant measure $d\mu(X_+^{4p,4q})$ on $X_+^{4p,4q}$ is expressed in parametrization (2.8) as

$$d\mu(X_+^{4p,4q}) = (\cosh\omega)^{4p-1}(\sinh\omega)^{4q-1}\, d\mu(X^{4p-1})\, d\mu(X^{4q-1})\, d\omega, \tag{2.27}$$

where $d\mu(X^{4p-1})$ and $d\mu(X^{4q-1})$ are the left-invariant measures on the compact subspaces X^{4p-1} and X^{4q-1} of $X_+^{4p,4q}$ and have been explicitly given in Paper I.

3. DEGENERATE IRREDUCIBLE UNITARY REPRESENTATIONS OF THE GROUPS $Sp(p,q)$

Let

$$X = G/K \tag{3.1}$$

be a homogeneous space where G is a semisimple Lie group and K a closed connected subgroup of G. Let $\tilde{X}$ be a homogeneous space homeomorphic to X. Then the group G acts transitively on $\tilde{X}$ and K is the stationary (little) group of $\tilde{X}$. Let $d\mu(\tilde{X})$ be a left-invariant measure on $\tilde{X}$. Let $\mathcal{H}(\tilde{X})$ be a Hilbert space of $L^2(\tilde{X}, \mu)$ type. The quasiregular representation of the group G on $\mathcal{H}(\tilde{X})$ is then defined as the mapping

$$\mathfrak{U}_g : \forall g \in G;\ g \to (\mathfrak{U}_g f)(x) = f(xg^{-1}),\quad f(x) \in \mathcal{H}(\tilde{X});\quad x \in \tilde{X}. \tag{3.2}$$

Let $\mathfrak{G}$ be the Lie algebra of G. Considering the infinitesimal transformations (3.2), we get the representation of the elements of $\mathfrak{G}$ as differential operators of the first order in coordinates of $\tilde{X}$ which are in general unbounded on $\mathcal{H}(\tilde{X})$. $\mathfrak{D}(\tilde{X})$ shall denote a dense manifold in $\mathcal{H}(\tilde{X})$, which is a common domain for all the generators of $\mathfrak{G}$.

In the case of our choice of homogeneous space (1.6) the group G is $Sp(p,q) \otimes Sp(1)$ and K is $Sp(p, q-1) \otimes Sp(1)$ or $Sp(p-1, q) \otimes Sp(1)$ in the case of $X_+^{4p,4q}$ or $X_-^{4p,4q}$, respectively. The algebra $\mathfrak{G}$ of $Sp(p,q) \otimes Sp(1)$ is formed by the set of generators

$$\begin{aligned}
\mathfrak{U}_{s,t}^+ &= \tfrac{1}{2}[z_s\partial_{-t} - z_{-s}\partial_t + z_t\partial_{-s} - z_{-t}\partial_s] \\
&\quad + \text{complex conjugate},\\
\mathfrak{U}_{s,t}^- &= \frac{1}{2i}[z_s\partial_{-t} + z_{-s}\partial_t + z_t\partial_{-s} + z_{-t}\partial_s] \\
&\quad + \text{complex conjugate},\\
\mathfrak{V}_{st}^+ &= \frac{1}{2i}[z_s\partial_t - z_{-s}\partial_{-t} + z_t\partial_s - z_{-t}\partial_{-s}] \\
&\quad + \text{complex conjugate},\\
\mathfrak{V}_{st}^- &= \tfrac{1}{2}[z_s\partial_t + z_{-s}\partial_{-t} - z_t\partial_s - z_{-t}\partial_{-s}] \\
&\quad + \text{complex conjugate}
\end{aligned} \tag{3.3}$$

for $1 \le s \le t \le p$ and $p+1 \le s \le t \le p+q$, together with the set of generators

$$\begin{aligned}
\mathfrak{S}_{s,t}^+ &= \frac{1}{2i}[z_s\tilde{\partial}_{-t} + z_{-s}\tilde{\partial}_t - \tilde{z}_t\partial_{-s} - \tilde{z}_{-t}\partial_s] + \text{c.c.},\\
\mathfrak{S}_{s,t}^- &= \tfrac{1}{2}[z_s\tilde{\partial}_{-t} - z_{-s}\tilde{\partial}_t - \tilde{z}_t\partial_{-s} + \tilde{z}_{-t}\partial_s] + \text{c.c.},\\
\mathfrak{C}_{s,t}^+ &= \tfrac{1}{2}[z_s\tilde{\partial}_t + z_{-s}\tilde{\partial}_{-t} + \tilde{z}_t\partial_s + \tilde{z}_{-t}\partial_{-s}] + \text{c.c.},\\
\mathfrak{C}_{s,t}^- &= \frac{1}{2i}[z_s\tilde{\partial}_t - z_{-s}\tilde{\partial}_{-t} - \tilde{z}_t\partial_s + \tilde{z}_{-t}\partial_{-s}] + \text{c.c.},
\end{aligned} \tag{3.4}$$

for $s = 1, \cdots, p$ and $t = p+1, \cdots, p+q$, where c.c. is the complex conjugate.

We call the generators $\mathfrak{U}_{s,t}^{\pm}$ and $\mathfrak{V}_{s,t}^{\pm}$ the "compact" ones, because they are generating the maximal compact subgroup $Sp(p) \otimes Sp(q)$ of $Sp(p,q)$, while the generators $\mathfrak{S}_{s,t}^{\pm}$ and $\mathfrak{C}_{s,t}^{\pm}$, which complete the total algebra, are called "noncompact." Furthermore, it is obvious from the commutation relations of the generators (3.3) and (3.4), which are presented in Appendix A, that the generators $\mathfrak{V}_{s,t}^{\pm}$ and $\mathfrak{C}_{s,t}^{\pm}$ together form a subalgebra $su(p,q)$ of $sp(p,q)$.

The remaining three operators which form the algebra $sp(1)_{p,q}$ are defined by

$$\begin{aligned}
\mathfrak{U}^+ &= \sum_{k=1}^{p+q}(z_k\partial_{-k}^* - z_{-k}^*\partial_k) + \text{c.c.},\\
\mathfrak{U}^- &= i\sum_{k=1}^{p+q}(z_k\partial_{-k}^* + z_{-k}^*\partial_k) + \text{c.c.},\\
\mathfrak{V} &= i\sum_{k=1}^{p+q}(z_k\partial_k - z_{-k}\partial_{-k}) + \text{c.c.}
\end{aligned} \tag{3.5}$$

In the above formulas z^* stands for the complex conjugate of z and ∂_k stands for $\partial/\partial z_k$. We choose for the domain $\mathfrak{D}(X_+^{4p,4q})$ of the generators of $\mathfrak{G}$ the linear manifold of the vectors $f(z) \in \mathcal{H}(X_+^{4p,4q})$ such that

$$f(z) = P(z_s, z_{-s}, z_s^*, z_{-s}^*)\exp\left\{-\sum_{s=1}^{p+q}(z_s z_s^* + z_{-s}z_{-s}^*)\epsilon_s\right\},$$

where $P(\cdots)$ is a polynomial in z_s, z_{-s}, z_s^*, z_{-s}^* $(s = 1, \cdots, p+q)$. Considering here formally $z_{\pm s}$ and $z_{\pm s}^*$ as independent variables, the proof[4] of the density $\mathfrak{D}(X_+^{4p,4q})$ in $\mathcal{H}(X_+^{4p,4q})$ can be repeated with only slight modifications. The domain $\mathfrak{D}(X_+^{4p,4q})$ is obviously invariant with respect to the action of $\mathfrak{G} \equiv sp(p,q) \oplus sp(1)_{p,q}$.

In order to obtain suitable carrier spaces for unitary irreducible representations of both G and $\mathfrak{G}$, let us consider the generalized Fourier transform of $\mathfrak{D}(X_+^{4p,4q})$ with respect to the eigenfunctions of the Laplace–Beltrami operator. Let us define

$$\chi_\alpha^\kappa = \langle f, V_\alpha^\kappa\rangle := \int_{X_+^{4p,4q}} f(\omega, \sigma_p, \tilde{\sigma}_q)[V_\alpha^\kappa(\omega; \sigma_p, \tilde{\sigma}_q)]^*\, d\mu(X_+^{4p,4q}), \tag{3.6}$$

where $V_\alpha^\kappa(\omega, \sigma_p, \tilde{\sigma}_q)$ is shorthand for the eigenfunction of $\Delta(X_+^{4p,4q})$, the full labeling of which corresponds to the decomposition

$$V_\alpha^\kappa(\omega, \sigma_p, \tilde{\sigma}_q) := \Omega_{L_p,\tilde{L}_q}^\kappa(\omega) \times Y_{\substack{M_p^-, M_{p-1}^-, \cdots, M_2^-, M_1^- \\ M_p^+, M_{p-1}^+, \cdots, M_2^+, M_1^+}}^{\substack{L_p, L_{p-1}, \cdots, L_2 \\ l_p, l_{p-1}, \cdots, l_2, l_1}}(\sigma_p) Y_{\substack{\tilde{M}_q^-, \cdots, \tilde{M}_2^-, \tilde{M}_1^- \\ \tilde{M}_q^+, \cdots, \tilde{M}_2^+, \tilde{M}_1^+}}^{\substack{\tilde{L}_q, \cdots, \tilde{L}_2 \\ \tilde{l}_q, \cdots, \tilde{l}_2, \tilde{l}_1}}(\tilde{\sigma}_q), \tag{3.7}$$

where $\kappa = L$ for the discrete part of the spectrum of

$$\Delta(X_+^{4p,4q}): \kappa \in DS(\Delta) := \{\lambda \mid \lambda = -L(L + 4p + 4q - 1), \quad L = 2p - 2q + 1 + K; K = 1, 2, \cdots\}$$

and $\kappa = \Lambda$ for the continuous part of the spectrum of

$$\Delta(X_+^{4p,4q}): \kappa \in CS(\Delta) := \{\lambda \mid \lambda = -2p - 2q + 1 + i\Lambda; \Lambda \geq 0\}.$$

We denote by A_κ the set of all possible values of indices which appear on the right-hand side of (3.7) with the exception of κ. The possible values of these indices are restricted by the conditions (2.26) and (2.27) of Paper I and by a condition (2.21) in the case of $\kappa \in DS(\Delta)$.

Now, the set of all sequences

$$\chi^\kappa := \{\chi_\alpha^\kappa \mid \alpha \in A_\kappa\} \tag{3.8}$$

spans a vector space which becomes a unitary space $\mathfrak{D}^\kappa(\mathcal{F})$ under the scalar product

$$(\chi^\kappa, \eta^\kappa) = \sum_{\alpha \in A_\kappa} \chi_\alpha^\kappa (\eta_\alpha^\kappa)^* = \sum_{\alpha \in A_\kappa} \langle f, V_\alpha^\kappa \rangle \langle g, V_\alpha^\kappa \rangle^* \tag{3.9}$$

if the condition

$$\|\chi^\kappa\| = (\chi^\kappa, \chi^\kappa)_{\mathfrak{D}(\mathcal{F})}^{\frac{1}{2}} < \infty \tag{3.10}$$

is satisfied.

The completion of $\mathfrak{D}^\kappa(\mathcal{F})$ with respect to the scalar product (3.9) is a Hilbert space $\mathcal{H}^\kappa(\mathcal{F})$. In this manner we can overcome the difficulty of non-square-integrability of the functions V_α^κ for $\kappa \in CS(\Delta)$. The unitary representations of the group $Sp(p, q)$ and its algebra $\mathfrak{sp}(p, q)$ are then defined as the mappings

$$Sp(p, q) \ni g \to \mathfrak{U}_g \chi^\kappa := \{\langle U_g f(z), V_\alpha^\kappa(z) \rangle \mid \alpha \in A_\kappa\} = \{\langle f(zg^{-1}), V_\alpha^\kappa(z) \rangle \mid \alpha \in A_\kappa\} \tag{3.11}$$

and

$$\mathfrak{sp}(p, q) \ni X_{ij}^{(s)} \to X_{ij}^{(s)} \chi^\kappa := \{\langle X_{ij}^{(s)} f(z), V_\alpha^\kappa \rangle \mid \alpha \in A_\kappa\}, \tag{3.12}$$

respectively. Here $f(z) \in \mathfrak{D}(X_+^{4p,4q})$ and we have introduced the denotation $X_{i,j}^{(s)}$ for any of the operators (3.3) and (3.4).

Keeping the indices L_p and $\tilde{L}_q$ fixed, we get a finite subset $A_\kappa^{L_p,\tilde{L}_q}$ of A_κ; the corresponding subsequences

$$\chi_{L_p,\tilde{L}_q}^\kappa := \{\chi_{L_p,\tilde{L}_q;\beta}^\kappa \mid \beta \in A_{L_p,\tilde{L}_q}^\kappa\} \tag{3.13}$$

span the subspaces $\mathfrak{D}_{L_p,\tilde{L}_q}^\kappa(\mathcal{F})$ of $\mathfrak{D}^\kappa(\mathcal{F})$.

It is easy to see from the formulas of Appendices I and II of Paper I, compared with those of Appendix B of the present paper, that the subspace $\mathfrak{D}_{L_p,\tilde{L}_q}^\kappa(\mathcal{F})$ remains invariant under the action of the maximal compact subalgebra $\mathfrak{sp}(p) \oplus \mathfrak{sp}(q) \oplus \mathfrak{sp}(1)_{p,q}$ of $\mathfrak{sp}(p, q) \oplus \mathfrak{sp}(1)_{p,q}$.

Moreover, as is shown in Paper I, the Laplace–Beltrami operator $\Delta(X^{4p-1})$ is proportional to the linear combination of Casimir operators of the algebras $\mathfrak{sp}(p)$ and $\mathfrak{sp}(1)_p$:

$$\Delta(X^{4p-1}) = C^{(2)}(\mathfrak{sp}(p)) - \tfrac{1}{2} C^{(2)}(\mathfrak{sp}(1)_p). \tag{3.14}$$

Let us consider the subspaces on which the eigenvalue $-\mathfrak{L}_p(\mathfrak{L}_p + 2)$ of $C^{(2)}(\mathfrak{sp}(1)_p)$ and the eigenvalue $M_{(p)}^+ = \sum_{i=1}^p M_i^+$ of the generator $\mathfrak{U}^+ \in \mathfrak{sp}(1)_p$ are fixed. Then it follows that those subspaces denoted by $\mathfrak{D}_{\substack{\mathfrak{L}_p, \tilde{\mathfrak{L}}_q \\ M_{(p)}^+, \tilde{M}_{(q)}^+}}^{L_p, \tilde{L}_q, \kappa}$ are invariant with respect to the action of the algebra $\mathfrak{sp}(p) \oplus \mathfrak{sp}(q)$.

Repeating the arguments of Paper I, we prove the irreducibility of these subspaces with respect to the action of the subalgebra $\mathfrak{sp}(p) \oplus \mathfrak{sp}(q)$ of $\mathfrak{sp}(p, q)$. With this in mind we can prove the following:

Proposition 1 (Irreducibility): The infinitesimal irreducible representations of the algebra $\mathfrak{sp}(p, q)$ are realized by the mapping (3.12) of $\mathfrak{D}_{\mathfrak{L},M^+}^\kappa(\mathcal{F})$ into itself.

Here, $\mathfrak{D}_{\mathfrak{L},M^+}^\kappa(\mathcal{F})$ is a Fourier transform of a common invariant domain of the generators $X_{i,j}^{(s)} \in \mathfrak{sp}(p, q)$ on which the Laplace–Beltrami operator $\Delta(X_+^{4p,4q})$, the second-order Casimir operator $C^{(2)}(\mathfrak{sp}(1)_{p,q})$ of $\mathfrak{sp}(1)_{p,q}$, and the generator $\mathfrak{U}^+ \in \mathfrak{sp}(1)_{p,q}$ are multiples of the identity operator, the corresponding eigenvalues being $\lambda(\kappa)$, $-\mathfrak{L}(\mathfrak{L} + 2)$ and $M^+(|M^+| \leq \mathfrak{L})$, respectively, with the relation (3.14) holding for $\Delta(X_+^{4p,4q})$, $C^{(2)}(\mathfrak{sp}(p, q))$, and $C^{(2)}(\mathfrak{sp}(1)_{p,q})$.

The invariance of $\mathfrak{D}_{\mathfrak{L},M^+}^\kappa(\mathcal{F})$ with respect to the action of $\mathfrak{sp}(p, q)$ generators is obvious from the fact that they commute with the three operators which define the space $\mathfrak{D}_{\mathfrak{L},M^+}^\kappa(\mathcal{F})$.

The structure of the space $\mathfrak{D}_{\mathfrak{L},M^+}^\kappa(\mathcal{F})$ with respect to the action of subalgebras of $\mathfrak{sp}(p, q)$ is determined

by the set of relations which have to be satisfied by the eigenvalues $\alpha \in A_\kappa$.

First of all, let us recall the relations from Paper I for the eigenvalues M_s^+, M_s^-, l_s, L_s $(s = 1, \cdots, p)$ and $\tilde{M}_s^+$, $\tilde{M}_s^-$, $\tilde{l}_s$, $\tilde{L}_s$ $(s = 1, \cdots, q)$.

We have

$$|M_s^\pm| = l_s - 2k, \qquad s = 1, \cdots, p, \quad (3.15)$$

$$|\tilde{M}_s^\pm| = \tilde{l}_s - 2k, \qquad s = 1, \cdots, q, \quad (3.16)$$

$$l_s + L_{s-1} = L_s - 2k \geq 0, \quad s = 2, \cdots, p, \quad (3.17)$$

$$\tilde{l}_s + \tilde{L}_{s-1} = \tilde{L}_s - 2k \geq 0, \quad s = 2, \cdots, q, \quad (3.18)$$

as well as

$$L_s \geq |M_{(s)}^+| \equiv \left| \sum_{t=1}^{s} M_t^+ \right| = \mathfrak{L}_s - 2k \geq 0, \qquad s = 1, \cdots, p, \quad (3.19)$$

and

$$\tilde{L}_s \geq |\tilde{M}_{(s)}^+| = \left| \sum_{t=1}^{s} \tilde{M}_t^+ \right| = \tilde{\mathfrak{L}}_s - 2k \geq 0, \qquad s = 2, \cdots, q. \quad (3.20)$$

To these relations arising from the compact subgroups must be added the relations

$$L_p + \tilde{L}_q \geq |M^+| = |M_{(p)}^+ + M_{(q)}^+| = \mathfrak{L} - 2k \geq 0. \quad (3.21)$$

Here k is a nonnegative integer for which the right-hand side is nonnegative.

The picture is completed by the relation (2.21) which restricts the possible values of L_p and $\tilde{L}_q$ for $\kappa \in DS(\Delta)$. The relations (3.19), (3.20), and (3.21) can be treated also as "vector coupling" relations:

$$\mathfrak{L}_s = \mathfrak{L}_{s-1} + \mathfrak{l}_s, \quad s = 1, \cdots, p, \quad (3.22)$$

$$\tilde{\mathfrak{L}}_s = \tilde{\mathfrak{L}}_{s-1} + \tilde{\mathfrak{l}}_s, \quad s = 1, \cdots, q, \quad (3.23)$$

and

$$\mathfrak{L} = \mathfrak{L}_p + \tilde{\mathfrak{L}}_q. \quad (3.24)$$

Thus the space $\mathfrak{D}^\kappa_{\mathfrak{L},M^+}(\mathcal{F})$ is decomposed to the direct sum of subspaces according to the formula

$$\mathfrak{D}^\kappa_{\mathfrak{L},M^+}(\mathcal{F}) = \bigoplus_{L_p} \bigoplus_{\tilde{L}_q} \bigoplus_{\mathfrak{L}_p} \bigoplus_{\tilde{\mathfrak{L}}_q} \bigoplus_{M_{(p)}^+} \mathfrak{D}^{\kappa\ L_p,\ \tilde{L}_q}_{\mathfrak{L}_p,\ \tilde{\mathfrak{L}}_q\ M_{(p)}^+,\ M_-^+ M_{(p)}^+}(\mathcal{F}'), \quad (3.25)$$

where the relations (3.19)–(3.24) and (2.21) are satisfied.

To prove the irreducibility of $\mathfrak{D}^\kappa_{\mathfrak{L},M^+}$ with respect to the algebra $\mathfrak{sp}(p,q)$, it is sufficient to prove that there exist operators $X_{ij}^{(s)} \in \mathfrak{sp}(p,q)$ such that any of the subspaces

$$\mathfrak{D}^{\kappa\ L_p,\tilde{L}_q;\mathfrak{L}_p,\tilde{\mathfrak{L}}_q}_{M_{(p)}^+,M_-^+M_{(p)}^+}(\mathcal{F}')$$

is connected with its nearest neighbors in (3.25) by the action of $X_{i,j}^{(s)}$. The generators $\mathcal{C}^\pm_{p,p+q}$ and $\mathcal{S}^\pm_{p,p+q}$ satisfy this condition, as is easy to see from formulas (B6) of Appendix B for the action of operators

$$E_{\pm e_p \mp e_{p+q}} = \pm \mathcal{C}^-_{p,p+q} + i\mathcal{C}^+_{p,p+q}$$

and

$$E_{\pm e_p \mp e_{p+q}} = \pm \mathcal{S}^+_{p,p+q} + i\mathcal{S}^-_{p,p+q},$$

which belong to the complexification C_{p+q} of $\mathfrak{sp}(p,q)$.

After completing the $\mathfrak{D}^{(\cdot)}(\mathcal{F})$ spaces to Hilbert spaces $\mathfrak{K}^{(\cdot)}(\mathcal{F})$, the irreducibility of a representation $D^L_{\mathfrak{L},M^+}$ and/or $C^\Lambda_{\mathfrak{L},M^+}$ in the case of $\mathfrak{K} \in DS(\Delta)$ and/or $\mathfrak{K} \in CS(\Delta)$, respectively, is proved in the same way as in Ref. 3.

Proposition 2 (Unitarity): The representation (3.12) for $f \in \mathfrak{D}^\kappa(X_+^{4p,4q})$ is norm preserving in $\mathfrak{D}^\kappa(\mathcal{F})$ and has a unique extension in $\mathfrak{K}^\kappa(\mathcal{F})$ for every $\kappa \in S(\Delta)$.

The proof completely follows that of Ref. 3. The unitarity is first proved for the group $Sp(p,q) \otimes Sp(1)_{p,q}$ and the unitarity of representations of $Sp(p,q)$ is then induced by that of $Sp(p,q) \otimes Sp(1)_{p,q}$.

Proposition 3: The irreducible unitary discrete (continuous) representations $D^L_{\mathfrak{L},M^+}(C^\Lambda_{\mathfrak{L},M^+})$ and $D^L_{\mathfrak{L},\tilde{M}^+}(C^\Lambda_{\mathfrak{L},\tilde{M}^+})$ are equivalent.

Let us consider the operators H, E_+, and E_- of $\mathfrak{sp}(1)_{p,q}$ algebra defined by

$$E_\pm = \mathfrak{U}^+ \pm i\mathfrak{U}^-, \quad H = -i\mathfrak{V}. \quad (3.26)$$

It follows from the commutation relations

$$[H, E_\pm] = \mp 2E_\pm \quad (3.27)$$

and for every functional $\chi^{\kappa,\mathfrak{L}}_{\tilde{M}^+} \in \mathfrak{D}^{\kappa,\mathfrak{L}}_{\tilde{M}^+}(\mathcal{F})$ that

$$[E_+]^{\frac{1}{2}(\tilde{M}^+ - M^+)} \chi^{\kappa,\mathfrak{L}}_{\alpha,\tilde{M}^+} \in \mathfrak{D}^{\kappa,\mathfrak{L}}_{M^+}(\mathcal{F}). \quad (3.28)$$

Thus we have for the discrete representations a relation of equivalence

$$[E_+]^{\frac{1}{2}(\tilde{M}^+ - M^+)} D^L_{\mathfrak{L},\tilde{M}^+} [E_-]^{\frac{1}{2}(\tilde{M}^+ - M^+)} = D^L_{\mathfrak{L},M^+} \quad (3.29)$$

and the same kind of relation for the continuous representations $C^\Lambda_{\mathfrak{L},M^+}$.

In Paper I we used the concepts of the highest-weight formalism to classify the UIR of the compact group $Sp(n)$. In the case of the noncompact groups this formalism has to be reformulated. There are, naturally, many ways of performing such a reformulation; for instance, one can use the Harish-Chandra[10]

[10] Harish-Chandra, Trans. Am. Math. Soc. **76**, 234 (1954); **76**, 26 (1954).

extreme vector formalism. This approach would, however, need a completely different parametrization of the $X_+^{4p,4q}$ manifold from that used in this paper. Nevertheless, it is possible to introduce a weight formalism based on the choice of the Cartan subalgebra spanned by the operators H_i $(i = 1, \cdots, p + q)$. The parametrization used has led to the decomposition formula (3.25), which is, in fact, a decomposition of the given representation $\mathfrak{D}_{\mathfrak{L}}^{\kappa}$ of $Sp(p, q)$ with respect to the content of representations of the maximal compact subgroup $Sp(p) \otimes Sp(q)$ of $Sp(p, q)$. Therefore it seems natural to define a characteristic vector of a given representation $\mathfrak{D}_{\mathfrak{L}}^{\kappa}$ of $Sp(p, q)$ as a vector which simultaneously belongs to the minimal possible highest weight with respect to the subgroup $Sp(p)$ and to the maximal (minimal) possible highest weight of the subgroup $Sp(q)$ in the case of discrete (continuous) IUR $D_{\mathfrak{L}}^{L}(C_{\mathfrak{L}}^{\Lambda})$ of $Sp(p, q)$. From irreducibility it follows that such a vector is unique. Obviously it can be used for generating any of the other basis vectors of the carrying space of the given UIR of $Sp(p, q)$ by subsequent action of the generators.

The full classification of representations of $Sp(p, q)$ obtained in this paper according to the above-mentioned formalism will be published separately. Generally speaking, there are six distinct classes of discrete representations which have different types of characteristic vectors. Three of them are characterized by only one integer number and can be considered as the most degenerate representations of $Sp(p, q)$. On the other hand, the continuous representations form a single class.

The results given in Secs. 2 and 3 are also valid for the space $X_-^{4p,4q}$ after interchanging $p \leftrightarrow q$ in all formulas and placing the tilde over the variables which did not previously have it and removing the tilde from those variables which had it. This yields another series of IUR of $Sp(p, q)$, which, however, possesses quite a similar structure to those discussed above.

4. CONCLUSIONS

The results obtained in Paper I and in Secs. 2 and 3 of the present paper can be summarized as follows:

(a) A set of discrete $(D_{M^{\mp}}^{L,\mathfrak{L}})$ and continuous $(C_{M^{\mp}}^{\Lambda,\mathfrak{L}})$ IUR of the group $Sp(p, q)$ characterized by two invariant numbers corresponding to $\Delta(X_{\pm}^{4p,4q})$ and $C^{(2)}(\mathfrak{sp}(p, q))$ eigenvalues has been constructed, L and $\mathfrak{L}$ being integer numbers of the same parity, otherwise uncorrelated and Λ an arbitrary positive real number.

(b) The decomposition of the representations $D_{M^{\mp}}^{L,\mathfrak{L}}$ and $C_{M^{\mp}}^{\Lambda,\mathfrak{L}}$ of $Sp(p, q)$ with respect to the compact subgroup $Sp(p) \otimes Sp(q)$ follows immediately from the decomposition (3.25).

(c) The basis functions of the corresponding Hilbert spaces are labeled by the eigenvalues of the set of $4p + 4q - 1$ commuting operators which is formed by the Laplace–Beltrami operator $\Delta(X_+^{4p,4q})$ of the basic space $X_+^{4p,4q}$, the two sets of Laplace–Beltrami operators defined on the compact subspaces $X^{4p-1}, X^{4(p-1)-1}, \cdots, X^7$ and $X^{4q-1}, X^{4(q-1)-1}, \cdots, X^7$. Finally, there is the set of the second-order Casimir operators of the subgroups, which appear in the following chains. First of all we have $Sp(p, q) \supset Sp(p) \otimes Sp(q)$. Now, for any compact subgroup of $Sp(p)$ and $Sp(q)$, the chains are

$$Sp(x) \supset Sp(x-1) \otimes Sp(1)_x, \quad x = p, p-1, \cdots, 2 \text{ or } x = q, q-1, \cdots, 2,$$

while

$$Sp(1)_x \supset U(1)_x, \quad x = p, p-1, \cdots, 1 \text{ or } x = q, q-1, \cdots, 1.$$

The generators of the subgroups $U(1)_x$ $(x = 1, \cdots, p + q)$ form the Cartan subalgebra of $\mathfrak{sp}(p, q)$.

(d) There exists a basis vector in the carrier space of every representation, uniquely defined by certain requirements. Using this "lowest" vector, any other vector of the whole carrier space of the given IUR can be constructed with the help of generators of the algebra $\mathfrak{sp}(p, q)$, and the IUR can be classified.

ACKNOWLEDGMENTS

The author would like to thank Professor Abdus Salam and Professor P. Budini as well as the IAEA for hospitality kindly extended to him at the International Centre for Theoretical Physics, Trieste, in 1965–1966 and in June 1967. It is a pleasure to thank Dr. R. Rączka for many valuable discussions and constant interest in the work as well as Professor L. Trlifaj, Dr. F. Janouch, and Dr. J. Fischer for some remarks and encouragement.

APPENDIX A: ALGEBRA OF $Sp(p, q) \otimes Sp(1)_{p,q}$

The algebra of $Sp(p, q)$ is generated by the operators (3.3) and (3.4), which have been obtained as infinitesimal operators of a quasiregular representation (3.11) of $Sp(p, q)$.

To write down the commutation relations fulfilled by the generators (3.3) and (3.4), we introduce a shorthand expression

$$[X^{(r)}, Y^{(r')}] = \tfrac{1}{2}[\epsilon_1\epsilon_2\epsilon_3\epsilon_4]Z^{(r'')} \tag{A1}$$

for

$$[X_{p,q}^{(r)}, Y_{s,t}^{(r')}] = \tfrac{1}{2}[\epsilon_1\delta_{q,s}Z_{p,t}^{(r'')} + \epsilon_2\delta_{p,s}Z_{q,t}^{(r'')} + \epsilon_3\delta_{q,t}Z_{p,s}^{(r'')} + \epsilon_4\delta_{p,t}Z_{q,s}^{(r'')}], \tag{A2}$$

where r, r', r'', ϵ_1, ϵ_2, ϵ_3, and ϵ_4 are either $+$ or $-$ signs and X, Y, Z, stand for any of the generators $\mathfrak{U}$, $\mathfrak{V}$, $\mathfrak{S}$, $\mathfrak{T}$ of $Sp(p,q)$.

The commutation relations are

$$\begin{aligned}
[\mathfrak{V}^-, \mathfrak{V}^-] &= \tfrac{1}{2}[+\,-\,-\,+]\mathfrak{V}^-;\\
[\mathfrak{V}^-, \mathfrak{T}^-] &= \tfrac{1}{2}[+\,-\,-\,+]\mathfrak{T}^-,\\
[\mathfrak{T}^-, \mathfrak{T}^-] &= -\tfrac{1}{2}[+\,-\,-\,+]\mathfrak{V}^-,
\end{aligned} \tag{A3}$$

$$\begin{aligned}
[\mathfrak{V}^\pm, \mathfrak{V}^+] &= \mp\tfrac{1}{2}[+\,\pm\,+\,\pm]\mathfrak{V}^\mp;\\
[\mathfrak{V}^\pm, \mathfrak{T}^+] &= \tfrac{1}{2}[+\,\pm\,+\,\pm]\mathfrak{T}^\mp,
\end{aligned} \tag{A4}$$

$$\begin{aligned}
[\mathfrak{T}^\pm, \mathfrak{V}^+] &= \pm\tfrac{1}{2}[+\,\pm\,+\,\pm]\mathfrak{T}^\mp;\\
[\mathfrak{T}^\pm, \mathfrak{T}^+] &= \tfrac{1}{2}[+\,\pm\,+\,\pm]\mathfrak{V}^\mp,
\end{aligned} \tag{A5}$$

$$\begin{aligned}
[\mathfrak{V}^\pm_\pm, \mathfrak{U}^+_\pm] &= \begin{matrix}+\\ \mp\end{matrix}\tfrac{1}{2}[+\,\pm\,+\,\pm]\mathfrak{U}^\mp_\pm;\\
[\mathfrak{V}^\pm_\pm, \mathfrak{S}^+_\pm] &= \begin{matrix}\mp\\ +\end{matrix}\tfrac{1}{2}[+\,\pm\,+\,\pm]\mathfrak{S}^\mp_\pm,
\end{aligned} \tag{A6}$$

$$\begin{aligned}
[\mathfrak{T}^\pm_\pm, \mathfrak{U}^+_\pm] &= \begin{matrix}+\\ \pm\end{matrix}\tfrac{1}{2}[+\,\pm\,+\,\pm]\mathfrak{S}^\mp_\pm;\\
[\mathfrak{T}^\pm_\pm, \mathfrak{S}^+_\pm] &= \begin{matrix}\pm\\ +\end{matrix}\tfrac{1}{2}[+\,\pm\,+\,\pm]\mathfrak{U}^\mp_\pm,
\end{aligned} \tag{A7}$$

$$\begin{aligned}
[\mathfrak{U}^\pm_\pm, \mathfrak{U}^+_\pm] &= -\tfrac{1}{2}[+\,+\,+\,+]\mathfrak{V}^\mp_\pm;\\
[\mathfrak{U}^\pm_\pm, \mathfrak{S}^+_\pm] &= \begin{matrix}\mp\\ \pm\end{matrix}\tfrac{1}{2}[+\,+\,+\,+]\mathfrak{T}^\mp_\pm;\\
[\mathfrak{S}^\pm_\pm, \mathfrak{S}^+_\pm] &= \begin{matrix}-\\ \pm\end{matrix}\tfrac{1}{2}[+\,+\,+\,+]\mathfrak{V}^\mp_\pm.
\end{aligned} \tag{A8}$$

It is easy to see that the commutation relations (A3) define an orthogonal $\mathfrak{so}(p,q)$ subalgebra and the relations (A3)–(A5) define a unitary $\mathfrak{su}(p,q)$ subalgebra of the algebra $\mathfrak{sp}(p,q)$.

Besides the generators (3.3) and (3.4), we further introduce a set of operators

$$H_k = -i\mathfrak{V}^+_{kk}, \quad k = 1, \cdots, p+q, \tag{A9}$$

$$E_{\pm\mathbf{e}_s\mp\mathbf{e}_t} = \mathfrak{V}^-_{st} \pm i\mathfrak{V}^+_{st}, \quad 1 \le s < t \le p \text{ or } p+1 \le s < t \le p+q, \tag{A10}$$

$$E_{\pm\mathbf{e}_s\mp\mathbf{e}_t} = \pm\mathfrak{T}^+_{st} + i\mathfrak{T}^-_{st}, \quad 1 \le s \le p,\ p+1 \le t \le p+q, \tag{A11}$$

$$E_{\pm\mathbf{e}_s\pm\mathbf{e}_t} = \mathfrak{U}^+_{st} \pm i\mathfrak{U}^-_{st}, \quad 1 \le s < t \le p \text{ or } p+1 \le s < t \le p+q, \tag{A12}$$

$$E_{\pm\mathbf{e}_s\pm\mathbf{e}_t} = \pm\mathfrak{S}^- + i\mathfrak{S}^+, \quad 1 \le s \le p,\ p+1 \le t \le p+q, \tag{A13}$$

$$E_{\pm 2\mathbf{e}_s} = 2^{-\frac{1}{2}}(\mathfrak{U}^+_{s,s} \pm i\mathfrak{U}^-_{s,s}), \tag{A14}$$

which fulfill the commutation relations

$$[H_k, H_l] = 0, \tag{A15}$$

$$[H_k, E_\alpha] = -\alpha_k E_\alpha, \tag{A16}$$

$$[E_\alpha, E_{-\alpha}] = \sum_k \alpha_k H_k. \tag{A17}$$

This basis differs from Weyl's standard basis only by factors $2^{-1}(p+q+1)^{-\frac{1}{2}}$ which would appear at each generator and on the right-hand sides of commutation relations (A15)–(A17) as a consequence of different value of the Killing form $B(E_\alpha, E_{-\alpha})$ for every root α; in our basis we have

$$B(E_\alpha, E_{-\alpha}) = -4(p+q+1), \tag{A18}$$

while in Weyl's standard basis $B(E_\alpha, E_{-\alpha}) = -1$ is required. We consider our basis to be more convenient for calculations because every root α is expressible in terms of $p+q$ unit vectors

$$\mathbf{e}_s \ (s = 1, \cdots, p+q),$$
$$\alpha \in \{\pm\mathbf{e}_s + \mathbf{e}_t, \pm\mathbf{e}_s \pm \mathbf{e}_t; 2\mathbf{e}_s \,|\, s, t = 1, \cdots, p+q\}.$$

Generally, the set of generators (A9)–(A14) is preferred in calculations to the generators (3.3) and (3.4) for the operators H_k ($k = 1, \cdots, p+q$) form a Cartan subalgebra and the generators $E_{\pm\alpha}$ act like the "step" operators on the functionals χ^κ_α defined by (3.8).

Because the explicit formulas of the generators (A9)–(A14) are complicated, we introduce at first the following denotations:

Let

$$\begin{aligned}
c_x &= \cos\vartheta_x; \quad s_x = \sin\vartheta_x,\\
C_x &= \cos\xi_x; \quad S_x = \sin\xi_x.
\end{aligned} \tag{A19}$$

(We insert a tilde over the respective symbols in the case of angles $\tilde\vartheta_x$ and $\tilde\xi_x$ for $x = p+1, \cdots, p+q$.)

Furthermore, let

$$C^\pm(\vartheta, \varphi) \equiv \mp\frac{i}{\cos\vartheta}\frac{\partial}{\partial\varphi} + \sin\vartheta\frac{\partial}{\partial\vartheta}, \tag{A20}$$

$$S^\pm(\vartheta, \varphi) \equiv \mp\frac{i}{\sin\vartheta}\frac{\partial}{\partial\psi} - \cos\vartheta\frac{\partial}{\partial\vartheta} \tag{A21}$$

and

$$\Gamma^\pm(\xi, \vartheta, \varphi) \equiv \tan\xi C^\pm(\vartheta, \varphi) + \cos\vartheta\frac{\partial}{\partial\xi}, \tag{A22}$$

$$\Sigma^\pm(\xi, \vartheta, \psi) \equiv \tan\xi S^\pm(\vartheta, \psi) + \sin\vartheta\frac{\partial}{\partial\xi}. \tag{A23}$$

Finally, let

$$\begin{aligned}
&\mathcal{A}^\pm_{x,y}(\xi_x, \cdots, \xi_y, \vartheta_x, \varphi_x)\\
&\quad\equiv c_x C_x \sum_{r=x+1}^{y} \frac{F^{x+1}_{r-1}}{F^{r+1}_y} C_r \frac{\partial}{\partial\xi_r}\\
&\qquad - \frac{1}{F^{x+1}_y}\left(\frac{1}{C_x} C^\pm(\vartheta_x, \varphi_x) + c_x S_x \frac{\partial}{\partial\xi_x}\right)
\end{aligned} \tag{A24}$$

and

$$\begin{aligned}
&\mathcal{B}^\pm_{x,y}(\xi_x, \cdots, \xi_y, \vartheta_x, \psi_x)\\
&\quad\equiv s_x C_x \sum_{r=x+1}^{y} \frac{F^{x+1}_{r-1}}{F^{r+1}_y} C_r \frac{\partial}{\partial\xi_r}\\
&\qquad - \frac{1}{F^{x+1}_y}\left(\frac{1}{C_x} S^\pm(\vartheta_x, \psi_x) + s_x S_x \frac{\partial}{\partial\xi_x}\right),
\end{aligned} \tag{A25}$$

where

$$F_x^y = \prod_{r=y}^{x} S_r. \tag{A26}$$

Then we can write the generators (A9)–(A14) in the following form:

(1) The generators of the compact subgroup are

$$H_k = i\left(\frac{\partial}{\partial\varphi_k} - \frac{\partial}{\partial\psi_k}\right), \tag{A27}$$

$$E_{\pm 2e_k} = 2^{-\frac{1}{2}} e^{\pm i(\varphi_k - \psi_k)}\left[\mp i \cot\vartheta_k \frac{\partial}{\partial\psi_k} \mp i\tan\vartheta_k \frac{\partial}{\partial\varphi_k} + \frac{\partial}{\partial\vartheta_k}\right], \tag{A28}$$

$$E_{\pm e_k \mp e_l} = -\tfrac{1}{2} e^{\pm i(\varphi_k - \varphi_l)}\left\{c_k C_k F_{l-1}^{k+1}\Gamma^{\mp}(\xi_l, \vartheta_l, \varphi_l) + c_l \frac{C_l}{S_l}\mathcal{A}_{k,l-1}^{\pm}(\xi_k, \cdots, \xi_l, \vartheta_k, \varphi_k)\right\} - \tfrac{1}{2} e^{\pm i(\psi_l - \psi_k)}\left\{s_k C_k F_{l-1}^{k+1}\Sigma^{\pm}(\xi_l, \vartheta_l, \psi_l) + s_l \frac{C_l}{S_l}\mathcal{B}_{k,l-1}^{\mp}(\xi_k, \cdots, \xi_{l-1}, \vartheta_k, \psi_k)\right\}, \tag{A29}$$

$$E_{\pm e_k \pm e_l} = -\tfrac{1}{2} e^{\pm i(\varphi_k - \psi_l)}\left\{c_k C_k F_{l-1}^{k+1}\Sigma^{\mp}(\xi_l, \vartheta_l, \psi_l) + s_l \frac{C_l}{S_l}\mathcal{A}_{k,l-1}^{\pm}(\xi_k, \cdots, \xi_l, \vartheta_k, \varphi_k)\right\} + \tfrac{1}{2} e^{\pm i(\varphi_l - \psi_k)}\left\{s_k C_k F_{l-1}^{k+1}\Gamma^{\pm}(\xi_l, \vartheta_l, \varphi_l) + c_l \frac{C_l}{S_l}\mathcal{B}_{k,l-1}^{\mp}(\xi_k, \cdots, \xi_{l-1}, \vartheta_k, \psi_k)\right\}. \tag{A30}$$

Here $1 \le k < l \le p$ or $p+1 \le k < l \le p+q$; in the latter case the variables should be taken with a tilde.

(2) The "noncompact" generators are

$$\begin{aligned} E_{\pm e_l \mp e_k} &= \pm\tfrac{1}{2} e^{\pm i(\varphi_l - \tilde{\varphi}_k)}\Big\{\tanh\omega\tilde{c}_k\tilde{C}_k\tilde{F}_{p+q}^{k+1}\mathcal{A}_{l,p}^{\pm}(\xi_l, \cdots, \xi_p, \vartheta_l, \varphi_l) \\ &\quad + \coth\omega c_l C_l F_p^{l+1}\mathcal{A}_{k,p+q}^{\mp}(\tilde{\xi}_k, \cdots, \tilde{\xi}_{p+q}, \tilde{\vartheta}_k, \tilde{\varphi}_k) \\ &\quad + \tilde{c}_k\tilde{C}_k\tilde{F}_{p+q}^{k+1}c_l C_l F_p^{l+1}\frac{\partial}{\partial\omega}\Big\} \\ &\quad \pm \tfrac{1}{2} e^{\pm i(\tilde{\varphi}_k - \psi_l)}\Big\{\tanh\omega\tilde{s}_k\tilde{C}_k\tilde{F}_{p+q}^{k+1}\mathcal{B}_{l,p}^{\mp}(\xi_l, \cdots, \xi_p, \vartheta_l, \psi_l) \\ &\quad + \coth\omega s_l C_l F_p^{l+1}\mathcal{B}_{k,p+q}^{\pm}(\tilde{\xi}_k, \cdots, \tilde{\xi}_{p+q}, \tilde{\vartheta}_k, \tilde{\psi}_k) \\ &\quad + \tilde{s}_k\tilde{C}_k\tilde{F}_{p+q}^{k+1}s_l C_l F_p^{l+1}\frac{\partial}{\partial\omega}\Big\}, \end{aligned} \tag{A31}$$

$$\begin{aligned} E_{\pm e_l \pm e_k} &= \pm\tfrac{1}{2} e^{\pm i(\varphi_l - \tilde{\varphi}_k)}\Big\{\tanh\omega\tilde{s}_k\tilde{C}_k\tilde{F}_{p+q}^{k+1}\mathcal{A}_{l,p}^{\pm}(\xi_l, \cdots, \xi_p, \vartheta_l, \varphi_l) \\ &\quad + \coth\omega c_l C_l F_p^{l+1}\mathcal{B}_{k,p+q}^{\mp}(\tilde{\xi}_k, \cdots, \tilde{\xi}_{p+q}, \tilde{\vartheta}_k, \tilde{\varphi}_k) \\ &\quad + \tilde{s}_k\tilde{C}_k\tilde{F}_{p+q}^{k+1}c_l C_l F_p^{l+1}\frac{\partial}{\partial\omega}\Big\} \\ &\quad \mp \tfrac{1}{2} e^{\pm i(\tilde{\varphi}_k - \psi_l)}\Big\{\tanh\omega\tilde{c}_k\tilde{C}_k\tilde{F}_{p+q}^{k+1}\mathcal{B}_{l,p}^{\mp}(\xi_l, \cdots, \xi_p, \vartheta_l, \psi_l) \\ &\quad + \coth\omega s_l C_l F_p^{l+1}\mathcal{A}_{k,p+q}^{\pm}(\tilde{\xi}_k, \cdots, \tilde{\xi}_{p+q}, \tilde{\vartheta}_k, \tilde{\varphi}_k) \\ &\quad + \tilde{c}_k\tilde{C}_k\tilde{F}_{p+q}^{k+1}s_l C_l F_p^{l+1}\frac{\partial}{\partial\omega}\Big\}. \end{aligned} \tag{A32}$$

Here $1 \le l \le p$ and $p+1 \le k \le p+q$.

The three generators of $Sp(1)_{p,q}$ are

$$H = -i\mathfrak{V} = i\sum_{k=1}^{p+q}\left(\frac{\partial}{\partial\varphi_k} + \frac{\partial}{\partial\psi_k}\right) \tag{A33}$$

and

$$\begin{aligned} E_{\pm} &= 2^{-\frac{1}{2}}(\mathfrak{U}^{+} \pm i\mathfrak{V}^{-}) \\ &= 2^{-\frac{1}{2}}\sum_{k=1}^{p+q} e^{\pm i(\varphi_k + \psi_k)}\left[\mp i\cot\vartheta_k\frac{\partial}{\partial\psi_k} \pm i\tan\vartheta_k\frac{\partial}{\partial\varphi_k} + \frac{\partial}{\partial\vartheta_k}\right]. \end{aligned} \tag{A34}$$

In the summation over $k = p+1, \cdots, p+q$ the tildes are obviously supposed over every variable.

APPENDIX B: THE ACTION OF THE GENERATORS OF $Sp(p,q)$ ON A BASIS SYSTEM OF THE REPRESENTATION SPACES

To obtain a proper orthogonal basis system of the representation space $\mathfrak{D}^{\kappa}_{\mathfrak{L},M^2}(\mathcal{F})$ defined in Sec. 3, one has to use, instead of the functions $\mathfrak{V}^{\kappa}_{\alpha}(\omega, \sigma_p, \tilde{\sigma}_q)$ defined by (3.7), a linear combination of them.

The choice of this linear combination is uniquely determined by the requirement of diagonalization of all second order Casimir operators besides the Laplace–Beltrami ones. Due to the relation (3.14) between these two types of invariant operators, the properties of a new basis are dictated by the second order Casimir operator of the group $Sp(1)$ which accompanies the symplectic group in the direct product. But these last operators behave exactly as the operators of the usual rotation group $SO(3)$ or the group $SU(2)$. Particularly, the functions $\mathfrak{V}^{\kappa}_{\alpha}(\omega, \sigma_p, \tilde{\sigma}_q)$ or the functionals χ^{κ}_{α}, more properly

written as

$$\chi_\alpha^\kappa \equiv \left\| \begin{matrix} L_p, & L_{p-1}, & \cdots, & L_2 \\ l_p, & l_{p-1}, & \cdots, & l_2, & l_1 \\ M_p^+, & M_{p-1}^+, & \cdots, & M_2^+, & M_1^+ \\ M_p^-, & M_{p-1}^-, & \cdots, & M_2^-, & M_1^- \end{matrix} \middle| \begin{matrix} \kappa \\ \tilde{L}_q, & \tilde{L}_{q-1}, & \cdots, & \tilde{L}_2 \\ \tilde{l}_q, & \tilde{l}_{q-1}, & \cdots, & \tilde{l}_2, & \tilde{l}_1 \\ \tilde{M}_q^+, & \tilde{M}_{q-1}^+, & \cdots, & \tilde{M}_2^+, & \tilde{M}_1^+ \\ \tilde{M}_q^-, & \tilde{M}_{q-1}^-, & \cdots, & \tilde{M}_2^-, & \tilde{M}_1^- \end{matrix} \right\|, \tag{B1}$$

behave with respect to the $C^{(2)}(Sp(1))$ operators as a tensor product basis. It then follows from the composition law (A33) and (A34) of the generators of $Sp(1)$ that a proper basis of $\mathfrak{D}^{\kappa}{}_{,M^+}(\mathcal{F})$ is

$$\left\{ \begin{matrix} L_p, & L_{p-1}, & \cdots, & L_2 \\ \mathfrak{L}_p, & \mathfrak{L}_{p-1}, & \cdots, & \mathfrak{L}_2 \\ l_p, & l_{p-1}, & \cdots, & l_2, & l_1 \\ M_p^-, & M_{p-1}^-, & \cdots, & M_2^-, & M_1^- \end{matrix} \middle| \begin{matrix} \kappa \\ \mathfrak{L} \\ \tilde{L}_q, & \tilde{L}_{q-1}, & \cdots, & \tilde{L}_2 \\ \mathfrak{L}_q, & \tilde{\mathfrak{L}}_{q-1}, & \cdots, & \tilde{\mathfrak{L}}_2 \\ \tilde{l}_q, & \tilde{l}_{q-1}, & \cdots, & \tilde{l}_2, & \tilde{l}_1 \\ \tilde{M}_q^-, & \tilde{M}_{q-1}^-, & \cdots, & \tilde{M}_2^-, & \tilde{M}_1^- \end{matrix} \right\}_{M^+}$$

$$= \sum_{M_{(p)}^+ = -\mathfrak{L}_p}^{\mathfrak{L}_p} (\mathfrak{L}_p M_{(p)}^+ \tilde{\mathfrak{L}}_q \tilde{M}_{(q)}^+ \,|\, \mathfrak{L} M^+) \sum_{M_{(p-1)}^+ = -\mathfrak{L}_{p-1}}^{\mathfrak{L}_{p-1}} \cdots \sum_{M_{(2)}^+ = -\mathfrak{L}_2 M_1^+ = -l_1}^{\mathfrak{L}_2} \sum^{l_1} \prod_{x=3}^{p} (\mathfrak{L}_{x-1} M_{(x-1)}^+ l_x M_x^+ \,|\, \mathfrak{L}_x M_{(x)}^+)$$

$$\times (l_1 M_1^+ l_2 M_2^+ \,|\, \mathfrak{L}_2 M_{(2)}^+) \sum_{M_{(q-1)}^+ = -\tilde{\mathfrak{L}}_{q-1}}^{\tilde{\mathfrak{L}}_{q-1}} \cdots \sum_{M_{(2)}^+ = -\tilde{\mathfrak{L}}_2 \tilde{M}_1^+ = -\tilde{l}_1}^{\tilde{\mathfrak{L}}_2} \sum^{\tilde{l}_1} \prod_{x=3}^{q} (\tilde{\mathfrak{L}}_{x-1} \tilde{M}_{(x-1)}^+ \tilde{l}_x \tilde{M}_x^+ \,|\, \tilde{\mathfrak{L}}_x \tilde{M}_{(x)}^+)$$

$$\times (\tilde{l}_1 \tilde{M}_1^+ \tilde{l}_2 \tilde{M}_2^+ \,|\, \tilde{\mathfrak{L}}_2 \tilde{M}_{(2)}^+) \left\| \begin{matrix} L_p, & L_{p-1}, & \cdots, & L_2 \\ l_p, & l_{p-1}, & \cdots, & l_2, & l_1 \\ M_p^+, & M_{p-1}^+, & \cdots, & M_2^+, & M_1^+ \\ M_p^-, & M_{p-1}^-, & \cdots, & M_2^-, & M_1^- \end{matrix} \middle| \begin{matrix} \kappa \\ \tilde{L}_q, & \tilde{L}_{q-1}, & \cdots, & \tilde{L}_2 \\ \tilde{l}_q, & \tilde{l}_{q-1}, & \cdots, & \tilde{l}_2, & \tilde{l}_1 \\ \tilde{M}_q^+, & \tilde{M}_{q-1}^+, & \cdots, & \tilde{M}_2^+, & \tilde{M}_1^+ \\ \tilde{M}_q^-, & \tilde{M}_{q-1}^-, & \cdots, & \tilde{M}_2^-, & \tilde{M}_1^- \end{matrix} \right\|, \tag{B2}$$

where $(l_1 m_1 l_2 m_2 \,|\, l_3 m_3)$ are the Clebsch-Gordan coefficients as defined, e.g., in Ref. 11 with $l = 2j$, etc. The summation in (B2) over $M_{(x)}^+$'s goes, naturally, in steps by two units. We recall here also the definition $M_{(x)}^+ = \sum_{s=1}^{x} M_s^+$. To describe completely the action of the generators of $Sp(p,q)$ on the above-defined basis functions, it is sufficient to give the formulas for the action of H_s, $E_{\pm 2e_s}$, $E_{\pm e_s \pm e_{s-1}}$, $E_{\pm e_s \mp e_{s-1}}$, as well as of two "noncompact" generators $E_{\pm e_p \pm e_q}$ and $E_{\pm e_p \mp e_q}$. What remains follows from the commutation relations or can be obtained in an inductive way. In order to save space, we omit in the following all the unnecessary indices which do not appear in the coefficients replacing them by dots. So we have

$$H_s \left\{ \begin{matrix} \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ \cdots M_s^- \cdots \end{matrix} \middle| \begin{matrix} \kappa \\ \mathfrak{L} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \end{matrix} \right\}_{M^+} = M_s^{\rightarrow} \left\{ \begin{matrix} \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ \cdots M_s^- \cdots \end{matrix} \middle| \begin{matrix} \kappa \\ \mathfrak{L} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \end{matrix} \right\}_{M^+}, \tag{B3}$$

$$E_{\pm 2e_s} \left\{ \begin{matrix} \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ \cdots\ l_s \ \cdots \\ \cdots M_s^- \cdots \end{matrix} \middle| \begin{matrix} \kappa \\ \mathfrak{L} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \end{matrix} \right\}_{M^+} = 2^{-\frac{1}{2}} [(l_s \mp M_s^-)(l_s + 2 \pm M_s^-)]^{\frac{1}{2}} \left\{ \begin{matrix} \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ \cdots\ l_s \ \cdots \\ M_s^- \pm 2 \cdots \end{matrix} \middle| \begin{matrix} \kappa \\ \mathfrak{L} \\ \cdots \\ \cdots \\ \cdots \\ \cdots \end{matrix} \right\}_{M^+}, \tag{B4}$$

[11] M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1961).

$$E_{\delta_s e_s+\delta_{s-1}e_{s-1}}\left(\begin{array}{ccc|c} & & & \kappa \\ & & & \mathfrak{L} \\ \hline \cdots & L_s, L_{s-1}, & \cdots & \cdots \\ \cdots & \mathfrak{L}_s, \mathfrak{L}_{s-1}, & \cdots & \cdots \\ \cdots & l_s, l_{s-1}, & \cdots & \cdots \\ \cdots & M_s^-, M_{s-1}^-, & \cdots & \cdots \end{array}\right)_{M^+}$$

$$= \mathcal{K}_{s,s-1}^{-1} \sum_{\delta l_s, \delta l_{s-1}, \delta L_{s-1}, \delta \mathfrak{L}_{s-1}=\pm 1} A_{s,s-1}(\delta_s, \delta_{s-1}) \left(\begin{array}{ccc|c} & & & \kappa \\ & & & \mathfrak{L} \\ \hline \cdots & L_s, L_{s-1}+\delta L_{s-1}, & \cdots & \cdots \\ \cdots & \mathfrak{L}_s, \mathfrak{L}_{s-1}+\delta \mathfrak{L}_{s-1}, & \cdots & \cdots \\ \cdots & l_s+\delta l_s, l_{s-1}+\delta l_{s-1}, & \cdots & \cdots \\ \cdots & M_s^-+\delta_s, M_{s-1}^-+\delta_{s-1}, & \cdots & \cdots \end{array}\right)_{M^+}, \quad \text{(B5)}$$

$$E_{\delta_p e_p+\delta_q e_{p+q}}\left(\begin{array}{ccc|c} & & & \kappa \\ & & & \mathfrak{L} \\ \hline L_p, & \cdots & \tilde{L}_q, & \cdots \\ \mathfrak{L}_p, & \cdots & \tilde{\mathfrak{L}}_q, & \cdots \\ l_p, & \cdots & \tilde{l}_q, & \cdots \\ M_p^-, & \cdots & \tilde{M}_q^-, & \cdots \end{array}\right)_{M^+}$$

$$= \mathcal{K}_{p,q}^{-1} \sum_{\delta L_p, \delta \tilde{L}_q, \delta \mathfrak{L}_p, \delta \tilde{\mathfrak{L}}_q, \delta l_p, \delta \tilde{l}_q=\pm 1} A_{p,q}(\delta_p, \delta_q) \left(\begin{array}{ccc|c} & & & \kappa \\ & & & \mathfrak{L} \\ \hline L_p+\delta L_p, & \cdots & \tilde{L}_q+\delta \tilde{L}_q, & \cdots \\ \mathfrak{L}_p+\delta \mathfrak{L}_p, & \cdots & \tilde{\mathfrak{L}}_q+\delta \tilde{\mathfrak{L}}_q, & \cdots \\ l_p+\delta l_p, & \cdots & \tilde{l}_q+\delta \tilde{l}_q, & \cdots \\ M_p^-+\delta_p, & \cdots & \tilde{M}_q^-+\delta_q, & \cdots \end{array}\right)_{M^+} \quad \text{(B6)}$$

Here we have abbreviated by δ_p and δ_q the signs ± 1 in the denotation of generators. The coefficients are

$$\mathcal{K}_{s,s-1} = 2^5[(l_s+1)(l_{s-1}+1)(L'_{s-1}+1)(\mathfrak{L}_{s-1}+1)]^{\frac{1}{2}}, \quad \text{(B7)}$$

$$\mathcal{K}_{p,q} = 2^7[(L'_p+1)(\tilde{L}'_q+1)(\mathfrak{L}_p+1)(\tilde{\mathfrak{L}}_q+1) \times (l_p+1)(\tilde{l}_q+1)]^{\frac{1}{2}}, \quad \text{(B8)}$$

$$A_{s,s-1}(\delta_s, \delta_{s-1}) = \delta_s\left[\frac{\delta_s+\delta_{s-1}}{2}\delta l_s + \frac{\delta_s-\delta_{s-1}}{2}\right] \times a^{\delta L_{s-1}, \delta l_s} b_{\delta L_{s-1}}^{\delta l_{s-1}} c_{\delta l_s}^{\delta_s} c_{\delta l_{s-1}}^{\delta_{s-1}} \times d_{\delta \mathfrak{L}_{s-1}}^{\delta l_{s-1}, \delta_{s-1}} f^{\delta \mathfrak{L}_{s-1}, \delta l_s}, \quad \text{(B9)}$$

$$A_{p,q}(\delta_p, \delta_q) = \left[\delta_p \frac{\delta_p+\delta_q}{2} + \delta \mathfrak{L}_q \frac{\delta_p-\delta_q}{2}\right] \times g^{\delta L_p, \delta \tilde{L}_q} b_{\delta L_p}^{\delta l_p} b_{\delta \tilde{L}_q}^{\delta \tilde{l}_q} c_{\delta l_p}^{\delta_p} c_{\delta \tilde{l}_q}^{\delta_q} \times d_{\delta \mathfrak{L}_p}^{\delta l_p, \delta_p} d_{\delta \tilde{\mathfrak{L}}_q}^{\delta \tilde{l}_q, \delta_q} f^{\delta \mathfrak{L}_p, \delta \tilde{\mathfrak{L}}_q}. \quad \text{(B10)}$$

The factors a, b, c, d, f, and g all have a very similar structure. So we have

$$a^{\delta L_{s-1}, \delta l_s} = \{(L'_s+1)^2 - [r(L'_{s-1}, l_s)]^2\}^{\frac{1}{2}}, \quad \text{(B11)}$$

$$b_{\delta L_x}^{\delta l_x} = \left\{\frac{[r(l_x, L'_x)]^2 - (L'_{x-1}+1)^2}{L'_x+1+\delta L_x}\right\}^{\frac{1}{2}}, \quad \text{(B12)}$$

$$c_{\delta l_x}^{\delta_x} = \left\{\frac{l_x+1+\delta l_x+\delta_x \cdot \delta l_x \cdot M_x^-}{l_x+1+\delta l_x}\right\}^{\frac{1}{2}}, \quad \text{(B13)}$$

$$d_{\delta \mathfrak{L}_x}^{\delta l_x, \delta_x} = \left[\delta_x \frac{\delta_x+\delta \mathfrak{L}_x}{2} + \delta l_x \frac{\delta_x-\delta \mathfrak{L}_x}{2}\right] \times \left\{\frac{[s(\mathfrak{L}_x, l_x)]^2 - (\mathfrak{L}_{x-1}+1)^2}{\mathfrak{L}_x+1+\delta \mathfrak{L}_x} \delta \mathfrak{L}_x \delta l_x\right\}^{\frac{1}{2}}, \quad \text{(B14)}$$

$$f^{\delta \mathfrak{L}_x, \delta \mathfrak{L}_y} = \{[[s(\mathfrak{L}_x, \mathfrak{L}_y)]^2 - (\mathfrak{L}+1)^2]\delta \mathfrak{L}_x \delta \mathfrak{L}_y\}^{\frac{1}{2}}, \quad \text{(B15)}$$

$$g^{\delta L_p, \delta \tilde{L}_q} = \{[r(\tilde{L}'_q, L'_p)]^2 - g^2\}^{\frac{1}{2}}, \quad \text{(B16)}$$

where

$$g = \begin{cases} L'+1 = L+2p+2q-1, & \kappa \in DS(\Delta), \\ i\Lambda, & \kappa \in CS(\Delta), \end{cases} \quad \text{(B17)}$$

while

$$r(l_1, l_2) = (l_1+\delta l_1) + \delta l_2(l_2+1) + 1 \quad \text{(B18)}$$

and

$$s(l_1, l_2) = \delta l_1(l_1+1) + \delta l_2(l_2+1) + 1. \quad \text{(B19)}$$

We have also introduced a convenient notation

$$L'_x = L_x + 2x - 2. \quad \text{(B20)}$$

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

New Methods for Reduction of Group Representations. III*

JOHN R. GABRIEL
Argonne National Laboratory, Argonne, Illinois

(Received 31 October 1968)

The reduction of a space S into its irreducible components $S = \sum S(\alpha, p)$ with respect to (w.r.t.) a group G is discussed in the case where G is the union of two subgroups G_1 and G_2, and S has already been reduced w.r.t. G_1 and G_2 separately.

1. INTRODUCTION

It has been pointed out in previous papers[1-3] that it is possible to use the commutator algebra $\mathcal{C}$ of a representation Γ of a group G in a space S to express S as the sum of irreducible spaces $S(\alpha, p)$, so that

$$S = \sum_{\alpha} \sum_{p=1}^{p_{\max}(\alpha)} S(\alpha, p),$$

where $S(\alpha, p)$ affords an irreducible representation Γ_α of G.

In this paper we discuss two things:

1. improved means of using $\mathcal{C}$ to reduce S, and
2. methods to construct $\mathcal{C}$ when G is the union of several subgroups each of whose representations in S has already been reduced. The situation where each subgroup is the Abelian group consisting of powers of a generator of G is a special case of this.

2. THE USE OF THE COMMUTATOR ALGEBRA

A. The Reduction

We need some preliminary lemmas.

Lemma 1: Let C be an arbitrary element of $\mathcal{C}$ and let σ be one of its eigenvalues. Call the space, which is spanned by eigenvectors of C belonging to σ, $S(\sigma)$. Then $S(\sigma)$ is invariant under G.

Proof: Let R be an element of G and x be a vector in $S(\sigma)$. Then

$$CRx = RCx = R\sigma x = \sigma Rx, \tag{2.1}$$

i.e., if x is in $S(\sigma)$, so is Rx.

Lemma 2: Any element of $\mathcal{C}$ not a multiple of $\mathbf{1}$ may be used to divide S into at least two subspaces, each invariant with respect to (w.r.t.) G.

Proof: If the eigenvectors of C span S, then our theorem is true, since there must be at least two distinct eigenvalues of C.

If the eigenvectors of C do not span S (for an example of this case consider the 2×2 matrix C where $c_{11} = 1$, $c_{12} = 1$, $c_{21} = 0$, $c_{22} = 1$), let the projection operator for each $S(\sigma)$ be $\epsilon(\sigma)$. Then $\epsilon = \sum_\sigma \epsilon(\sigma)$ is in $\mathcal{C}$. Because eigenvectors belonging to different eigenvalues must be linearly independent, the $\epsilon(\sigma)$ are disjoint, i.e.,

$$\epsilon(\sigma)\epsilon(\sigma') = \delta_{\sigma\sigma'}\epsilon(\sigma); \tag{2.2}$$

and so $\epsilon^2 = \epsilon$, i.e., ϵ is a projection operator. Since $\epsilon^2 = \epsilon$, $\bar{\epsilon} = \mathbf{1} - \epsilon$ is also a projection operator, i.e., $\bar{\epsilon}^2 = \bar{\epsilon}$.

The decomposition

$$\mathbf{1} = \bar{\epsilon} + \sum \epsilon(\sigma) \tag{2.3}$$

decomposes S into at least two subspaces if there is at least one $\epsilon(\sigma)$ not equal to $\mathbf{1}$.

Since the eigenvectors of C do not span S, C is not a multiple of $\mathbf{1}$, but there exists some σ such that $(C - \sigma\mathbf{1})$ is singular.

Since $(C - \sigma\mathbf{1})$ is singular there exists at least one vector orthogonal to every row of $(C - \sigma\mathbf{1})$, i.e., there exists at least one eigenvector belonging to σ.

It follows that if $\mathcal{C}$ contains matrices other than multiples of $\mathbf{1}$, then there is always a nontrivial decomposition of S given by

$$\mathbf{1} = \sum_{\sigma} \epsilon(\sigma), \tag{2.4}$$

$$S = \sum_{\sigma} S(\sigma), \tag{2.5}$$

where one of the $\epsilon(\sigma)$ may be the $\bar{\epsilon}$ of lemma 2.

Each space $S(\sigma)$ is invariant w.r.t. G. Any element R of G may also be decomposed

$$R = \sum_{\sigma} R_\sigma, \tag{2.6}$$

where

$$R_\sigma = \epsilon_\sigma R \epsilon_\sigma \tag{2.7}$$

and

$$\epsilon_\sigma R \epsilon_{\sigma'} = \delta_{\sigma\sigma'} R_\sigma. \tag{2.8}$$

If $\mathbf{1}$ and C of lemma 2 do not span $\mathcal{C}$ then there exists C_1, a linearly independent element of $\mathcal{C}$.

Because of (2.3),

$$C_1 = (\sum \epsilon_\sigma) C_1 (\sum \epsilon_\sigma), \tag{2.9}$$

i.e.,

$$C_1 = \sum C_{1\sigma\sigma'}, \tag{2.10}$$

$$C_{1\sigma\sigma'} = \epsilon_\sigma C_1 \epsilon_{\sigma'}. \tag{2.11}$$

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

[1] J. R. Gabriel, J. Math. Phys. **5**, 494 (1964).
[2] J. R. Gabriel, J. Chem. Phys. **43**, S265 (1965).
[3] J. R. Gabriel, J. Math. Phys. **9**, 973 (1968).

Substituting (2.10) and (2.6) and using (2.2) in

$$RC_1 = C_1R, \tag{2.12}$$

we find that

$$R_\sigma C_{1\sigma\sigma} = C_{1\sigma\sigma}R_\sigma, \tag{2.13}$$

$$R_\sigma C_{1\sigma\sigma'} = C_{1\sigma\sigma'}R_{\sigma'}. \tag{2.14}$$

But Eq. (2.14) is just $CR = RC$ over again in $S(\sigma)$ and shows that either

$$C_{1\sigma\sigma} = \lambda\mathbf{1} \tag{2.15}$$

or that the eigenvectors of $C_{1\sigma\sigma}$ show a subdivision of $S(\sigma)$ into invariant subspaces $S(\sigma_1)$ w.r.t. G., and for each of the new subspaces $S(\sigma_1)$,

$$C_{1\sigma_1\sigma_1} = \lambda(\sigma_1)\mathbf{1}. \tag{2.16}$$

This process can be continued until the matrices which span $\mathfrak{C}$ have been exhausted. As soon as this is the case,

$$C_{\sigma\sigma} = \lambda(\sigma, C)\mathbf{1} \tag{2.17}$$

for every C and every σ, and every S_σ is irreducible as well as invariant, for if not there would be some C for which

$$C_{\sigma\sigma} \neq \lambda(\sigma, C)\mathbf{1}. \tag{2.18}$$

B. Spaces Which Afford Equivalent Irreducible Representations

Now we must turn our attention to (2.14). If

$$C_{\sigma\sigma'} \neq 0, \tag{2.19}$$

then (2.14) and Schur's lemma show that $C_{\sigma\sigma'}$ is square and nonsingular so that (2.14) becomes

$$R_{\sigma'} = C_{\sigma\sigma'}^{-1}R_\sigma C_{\sigma\sigma'} \tag{2.20}$$

for each R in G.

Therefore $S(\sigma)$ and $S(\sigma')$ afford equivalent irreducible representations (IR's) and $C_{\sigma\sigma'}$ is the change of basis in $S(\sigma')$ which makes $S(\sigma)$ and $S(\sigma')$ afford the same representation.

3. CONSTRUCTING $\mathfrak{C}$

Suppose that G_1 and G_2 are groups having representations Γ_1 and Γ_2 in some space S.

Suppose the decomposition of S w.r.t. G_1 is

$$S = \sum_{\alpha_1} \sum_{p_1=1}^{p_{\max}(\alpha_1)} S(\alpha_1, p_1) \tag{3.1}$$

and w.r.t. G_2

$$S = \sum_{\alpha_2} \sum_{p_2=1}^{p_{\max}(\alpha_2)} S(\alpha_2, p_2). \tag{3.2}$$

Each of the $p_{\max}(\alpha)$ spaces $S(\alpha, p)$ labeled by a given α affords the same IR Γ_α. $S(\alpha, p)$ has dimension n_α and its base vectors are

$$x(\alpha, p, i) \quad i = 1, \cdots, n_\alpha. \tag{3.3}$$

Define

$$e_{pq}^\alpha = \sum_i x^\dagger(\alpha, p, i)x(\alpha, q, i), \tag{3.4}$$

where $x^\dagger$ is the Hermitian conjugate of x.

Then Schur's lemma shows that an arbitrary element of the commutator algebra is[1–3]

$$C = \sum_\alpha \sum_{pq} c_{pq}^\alpha e_{pq}^\alpha. \tag{3.5}$$

Applying this to the groups G_1 and G_2 if C_1 and C_2 belong to $\mathfrak{C}_1$ and $\mathfrak{C}_2$,

$$C_1 = \sum_{\alpha_1} \sum_{p_1q_1} c_{p_1q_1}^{\alpha_1} e_{p_1q_1}^{\alpha_1}, \tag{3.6}$$

$$C_2 = \sum_{\alpha_2} \sum_{p_2q_2} c_{p_2q_2}^{\alpha_2} e_{p_2q_2}^{\alpha_2}. \tag{3.7}$$

Now if C is in $\mathfrak{C}$ the commutator of G, the union of G_1 and G_2, C must be in both C_1 and C_2, i.e., it is described by coefficients $c_{p_1q_1}^{\alpha_1}$ or $c_{p_2q_2}^{\alpha_2}$ which are solutions of

$$\sum_{\alpha_1} \sum_{p_1q_1} c_{p_1q_1}^{\alpha_1} e_{p_1q_1}^{\alpha_1} = \sum_{\alpha_2} c_{p_2q_2}^{\alpha_2} e_{p_2q_2}^{\alpha_2}. \tag{3.8}$$

Now C_1 of (3.6) is a vector in a linear vector space whose base vectors are the $e_{p_1q_1}^{\alpha_1}$, and similarly for C_2 of (3.7).

If the scalar product of two matrices e_1 and e_2 is defined by

$$e_1 \cdot e_2 = \mathrm{Tr}\,(e_1^\dagger e_2), \tag{3.9}$$

it fulfills all the requirements for a scalar product. Moreover if the e_{pq}^α are redefined by

$$e_{pq}^\alpha = (n_\alpha)^{-\frac{1}{2}} \sum_i x^\dagger(\alpha, p, i)x(\alpha, q, i), \tag{3.10}$$

the $e_{p_1q_1}^{\alpha_1}$ are an orthonormal basis for C_1 and similarly for C_2. Thus (3.8) may be rewritten

$$\sum a_i u_i = \sum b_j v_j, \tag{3.11}$$

where the u_i and v_j are sets of orthonormal base vectors spanning different subspaces of the set of all $n \times n$ matrices.

Equation (3.11) can be written as two simultaneous matrix equations for the coefficients

$$a_i = \sum (u_i \cdot v_j)b_j, \tag{3.12}$$

$$b_j = \sum (v_j \cdot u_i)a_i, \tag{3.13}$$

by writing

$$t_{ij} = (u_i \cdot v_j); \tag{3.14}$$

then

$$(v_j \cdot u_i) = t_{ji}^*,$$

and (3.12) and (3.13) may be written

$$A = TB, \tag{3.15}$$

$$B = T^\dagger A. \tag{3.16}$$

Eliminating B,

$$A = TT^\dagger A, \tag{3.17}$$

i.e., the vectors common to both spaces are eigenvectors of $TT^\dagger$ belonging to the eigenvalue 1.

4. REFINEMENTS AND EXTENSIONS

A. Statement of the Problem

The methods developed in Secs. 2 and 3 are obviously usable, powerful, and well suited to implementation on an electronic computer. However, if the dimension of the space S is large enough, the program will be too big for the computer.

It is therefore worthwhile to look for ways in which the processes, particularly those of Sec. 2, may be condensed. Moreover, a closer examination of the methods of this paper and their relationship with those proposed in earlier papers may give further insight into the structure of S.

For the remainder of this paper we shall restrict ourselves to consideration of a group $G(n)$ defined by n generators $R_1, R_2, \cdots, R_n$. If $G(i)$ is the group defined by the first i generators, $G(n) \supset G(n-1) \supset G(n-2) \supset \cdots \supset G(1) \supset G(0)$, where $G(0)$ is the unit matrix and $G(1) \cdots G(n)$ a sequence of subgroups.

We shall assume that S has been reduced w.r.t. $G(n-1)$ according to

$$S = \sum_{\alpha} \sum_{p} S(\alpha, p) \tag{4.1}$$

and we wish to inquire how R_n affects the spaces $S(\alpha, p)$. Some may remain invariant; some may become parts of a larger space which is reducible w.r.t. $G(n-1)$, but not w.r.t. $G(n)$, or perhaps two spaces $S(\alpha, 1)$ and $S(\alpha, 2)$ which afford the same representation of $G(n-1)$ may afford inequivalent representations of $G(n)$, for example.

Assuming we know how to reduce S w.r.t. $G(n-1)$, we may use this knowledge to reduce S with regard to $G(n)$ in the following way. Since $G(n-1)$ is a subgroup of $G(n)$, any basis for S which displays its reduction w.r.t. $G(n)$ must display a reduction w.r.t. $G(n-1)$. If we require the basis in S which displays the reduction of $G(n)$ to display the known reduction of $G(n-1)$, then the mapping P of the basis for $G(n)$ onto the known basis for $G(n-1)$ must obey $P^{-1}\Gamma(n-1)P = \Gamma(n-1)$, i.e., P belongs to the commutator algebra of $\Gamma(n-1)$. This is a very helpful restriction since if $S(\alpha, p)p = 1, \cdots, p_{\max}(\alpha)$ are the spaces which afford Γ_α of $G(n-1)$ and

$$S_\alpha = \sum_{p=1}^{p_{\max}(\alpha)} S(\alpha, p), \tag{4.2}$$

then S_α *must be invariant under* P.

This suggests that we may be able to determine P by considering the S_α of (4.2) one by one. What this means in terms of P is as follows: If $e(\alpha, p, q)$ is as defined by (3.4) and we write

$$\epsilon_\alpha = \sum_{p} e(\alpha, p, p), \tag{4.3}$$

then since P leaves S_α invariant,

$$\epsilon_\alpha P \epsilon_{\alpha'} = \delta_{\alpha\alpha'} P_\alpha, \tag{4.4}$$

where P_α is the submatrix of P which operates in S_α. Since $\sum_\alpha \epsilon_\alpha = \mathbf{1}$,

$$P = \sum P_\alpha. \tag{4.5}$$

To see what is the function of the matrices P_α and how we might determine them, we need two lemmas.

Lemma 1: Let $S(\alpha, 1)$ and $S(\alpha, 2)$ both afford the same representation Γ_α of G. Let

$$v_1 = \sum_i a_i x(\alpha, 1, i) \tag{4.6}$$

and

$$v_2 = \sum_i a_i x(\alpha, 2, i) \tag{4.7}$$

[i.e., v_1 and v_2 are corresponding vectors in $S(\alpha, 1)$ and $S(\alpha, 2)$, and $\sum_i x^\dagger(\alpha, 1, i)x(\alpha, 2, i)$ belongs to $\mathfrak{C}$].

Let

$$v = \lambda v_1 + \mu v_2. \tag{4.8}$$

Then the vectors Tv as T varies over G span a proper invariant subspace of $S = S(\alpha, 1) + S(\alpha, 2)$ whose base vectors are

$$x(\alpha, i) = \lambda x(\alpha, 1, i) + \mu x(\alpha, 2, i), \tag{4.9}$$

which is invariant w.r.t. G and affords the irreducible representation Γ_α.

Proof: Let

$$e^\alpha_{ij} = \frac{n_\alpha}{g} \sum_G \Gamma^\alpha_{ij}(T^{-1})T; \tag{4.10}$$

then it is well known[4] that

$$e^\alpha_{ij} x(\alpha, k) = x(\alpha, i)\delta_{jk}. \tag{4.11}$$

Then it is easy to show that for some j_0,

$$v_{\alpha i} = e^\alpha_{ij_0} v \tag{4.12}$$

is nonzero and that the n_α vectors

$$v_{\alpha i}, \quad i = 1, \cdots, n_\alpha \tag{4.13}$$

span the space whose base vectors are (4.9). But

$$v_{\alpha i} = \frac{n_\alpha}{g} \sum \Gamma^\alpha_{ij}(T^{-1})Tv, \tag{4.14}$$

which is a linear combination of the vectors Tv.

This proves the lemma.

Note that the transformation (4.9) commutes with $G(n-1)$.

Lemma 2: If S_α and S_β afford inequivalent IR's of G, then S_α and S_β are the only invariant subspaces of $S = S_\alpha + S_\beta$ w.r.t. G.

Proof: Is similar to lemma 1.

These two lemmas show how R_n affects the basis which reduces $\Gamma(n-1)$, the representation of $G(n-1)$ in S. For example, if S_α and S_β afford inequivalent IR's of $G(n-1)$, each occurs only once, and there exist x_α and x_β in S_α and S_β such that

$$x_\beta = R_n x_\alpha. \tag{4.15}$$

Then S_β cannot be invariant w.r.t. $G(n)$ and by lemma 2, $S_\alpha + S_\beta$ must be irreducible w.r.t. $G(n)$.

[4] H. Weyl, *Group Theory of Quantum Mechanics* (Dover Publications, Inc., New York, 1931).

Of course $S_\alpha + S_\beta$ may not be invariant, it may be coupled to $S_{\alpha'}$ by R_n, by an equation like (4.15), and so on and so forth.

However, if we have two spaces $S(\alpha, 1)$ and $S(\alpha, 2)$ which afford the same representation, together with S_β and there exist $x_{\alpha 1}$, $x_{\alpha 2}$, x_β, $x_{\beta'}$ such that

$$x_\beta = R_n x_{\alpha 1}, \tag{4.16}$$

$$x_{\beta'} = R_n x_{\alpha 2}, \tag{4.17}$$

then our first thought is that $S(\alpha, 1) + S(\alpha, 2) + S(\beta)$ is irreducible, but this is not necessarily so. There might be some space S'_α whose base vectors are

$$x'(\alpha, i) = \lambda x(\alpha, 1, i) + \mu x(\alpha, 2, i), \tag{4.18}$$

such that there are no nonzero matrix elements of R_n between $S_{\alpha'}$ and S_β to make $S_{\alpha'}$ not invariant according to lemma 2.

In this case the transformation (4.18) is a simple example of a P_α in the sense of (4.5).

This explains what the problem is.

B. The Process of Reduction

This divides into two parts:

(1) finding the basis changes P_α of Eq. (4.5);

(2) finding which spaces S_β are coupled to the new basis for Γ_α found in Part (1) by R_n.

Part (1) is done by extending Sec. 2. Let C be an element of the commutator algebra $\mathcal{C}(n)$ of $G(n)$ and let $S_\alpha = \sum_p S(n-1, \alpha, p)$. Then since C is, *a fortiori*, in $\mathcal{C}(n-1)$, C leaves each S_α invariant. Thus

$$C = \sum_\alpha C_\alpha, \tag{4.19}$$

where

$$C_\alpha = \epsilon_\alpha C \epsilon_\alpha \tag{4.20}$$

analogously to (4.5).

Just as (3.5) expresses C in terms of the e^α_{pq} for $\Gamma(n-1)$, so

$$C_\alpha = \sum_{pq} C^\alpha_{pq} e^\alpha_{pq}. \tag{4.21}$$

Note that the sum over α in (3.5) is missing from (4.21).

Equation (4.21) expresses the condition that C_α is in $\mathcal{C}(n-1)$. If C_α also commutes with R_n, then C_α is in $\mathcal{C}(n)$. But because $S_\alpha = \sum_p S(\alpha, p)$ is invariant w.r.t. C_α, the process of Sec. 2 can be applied to S_α by itself. This greatly reduces the order of the eigenvalue problems that lead to Eqs. (2.1)–(2.8). The group G_2 of Sec. 3 is just the Abelian group generated by R_n, and its commutator algebra can be obtained from the eigenvectors of R_n (if the eigenvectors do not span S, then tricks like those in Sec. 2A must be used).

If $p_{\max}(\alpha)$ is the number of times Γ_α appears in S_α, then $TT^\dagger$ of 3.117 is $p_{\max}(\alpha) \times p_{\max}(\alpha)$.

Having used C_α to find a basis in S_α which takes the greatest possible advantage of lemma 1 of Sec. 4 for each α value in S,then we use lemma 2 to see which are the inequivalent spaces coupled by R_n to make larger spaces which are reducible w.r.t. $G(n-1)$ but not w.r.t. $G(n)$.

C. Comments on Secs. 4A and 4B and an Alternative Method

The preceding is most closely related to the second paper in this series, where linear operators are treated as sums of dyadics rather than being expressed in any special basis. In particular, to express any of the equations of Sec. 3 or Sec. 4 in matrix form, the same basis must be chosen for the expression of each side of the equation.

However, given the situation described in Sec. 3, there are two "natural" bases; the first,

$$x(\alpha_1, p_1, i_1),$$

is appropriate to G_1, and the second,

$$x(\alpha_2, p_2, i_2),$$

is appropriate to G_2.

The transformation H which transforms each basis vector $x(\alpha_1, p_1, i_1)$ into a corresponding vector $x(\alpha_2, p_2, i_2)$ may be written

$$H = \sum_{\alpha_1 \alpha_2 p_1 p_2 i_1 i_2} x(\alpha_2, p_2, i_2) x^\dagger(\alpha_1, p_1, i_1). \tag{4.22}$$

The matrix of H in the basis $x(\alpha_1, p_1, i_1)$ is

$$H(\alpha_2, p_2, i_2, \alpha_1, p_1, i_1) = x^\dagger(\alpha_1, p_1, i_1) x(\alpha_2, p_2, i_2). \tag{4.23}$$

If

$$C_1 = \sum_{\alpha_1 p_1 q_1} c^{\alpha_1}_{1 p_1 q_1} \epsilon(\alpha_1, p_1, q_2) \tag{4.24}$$

is a member of $\mathcal{C}_1$, its matrix representative in the $x(\alpha_1, p_1, i_1)$ basis is

$$x^\dagger(\alpha_1, p_1, i_1) C_1 x(\alpha'_1, p'_1, i'_1) = \delta_{\alpha_1 \alpha'_1} \delta_{i_1 i'_1} c^{\alpha_1}_{1 p_1 q_1}.$$

If C_1 is not only an element of $\mathcal{C}_1$ but also of $\mathcal{C}_2$, then its matrix element in the $x(\alpha_2, p_2, i_2)$ basis is

$$\delta_{\alpha_2 \alpha'_2} \delta_{i_2 i'_2} c^{\alpha_2}_{2 p_2 q_2}. \tag{4.25}$$

These must be related by the linear transformation H, i.e.,

$$HC_1 H^{-1} = C_2$$

or

$$HC_1 = C_2 H$$

or

$$\sum_{\alpha_1 p_1} H(\alpha_2, p_2, i_2; \alpha_1, p_1, i_1) c^{\alpha_1}_{1 p_1 q_1} = \sum_{\alpha_2 q_2} c^{\alpha_2}_{2 p_2 q_2} H(\alpha_2, q_2, i_2; \alpha_1, q_1, i_1). \tag{4.26}$$

This equation may be used instead of Sec. 3 to determine $\mathcal{C}$, although Sec. 3 is usually considerably easier to work with. In this context it should be noted that

the matrix t_{ij} of (3.14) may be expressed simply in terms of H of (4.22).

5. AN EXAMPLE

To make it easier for the reader to follow the arguments and to help resolve any ambiguities, consider the following example.

Let (x, y, z) be three variables which transform under the group defined by

$$R_4: (x, y, z) \to (y, -x, z), \tag{5.1}$$

$$R_2: (x, y, z) \to (z, -y, x). \tag{5.2}$$

Let S be the 6-dimensional space of all 2nd-degree polynomials in (x, y, z). The six monomials

$$x^2\ y^2\ z^2\ xy\ yz\ zx$$

form a basis for S.

The group defined by R_4 and R_2 is the tetrahedral group T and the space S affords a reducible representation of the cubic group. Let us apply the techniques of this paper to finding the irreducible subspaces of S w.r.t. T.

Because the methods of Sec. 2 and Sec. 3 are awkward to write out in a hand-calculated example since the methods were devised for use on a digital computer, we shall take some short cuts which eliminate the need to print many matrices.

Nevertheless, the hand calculation given here provides a useful clue to the ideas behind the rest of the paper.

We choose eigenvectors of R_4 for our basis set. They are

$$\begin{aligned} &(x^2 + y^2)/\sqrt{2}, \\ &z^2, \\ &(x^2 - y^2)/\sqrt{2}, \\ &xy, \\ &z(x + iy)/\sqrt{2}, \\ &z(x - iy)/\sqrt{2}. \end{aligned} \tag{5.3}$$

They are related to x^2, y^2, z^2, xy, yz, zx by a unitary transformation which makes R_4 diagonal.

The matrices R_2 and R_4 in this basis are shown in Eqs. (5.6a) and (5.6b). C_4 in Eq. (5.6c) is a general element of the commutator algebra of R_4.

We must now find the conditions on the coefficients c^{α}_{pq} in

$$C_4 = \sum_{\alpha pq} c^{\alpha}_{pq} e^{\alpha}_{pq}, \tag{5.4}$$

which make it commute with R_2.

Instead of using the techniques of Sec. 3, it is simpler in this case to solve the equation

$$C_4 R_2 = R_2 C_4 \tag{5.5}$$

for the c^{α}_{pq}.

The products C_4R_2 and R_2C_4 are displayed in Eqs. (5.7a), (5.7b).

If all of the equations for c^1_{11}, c^1_{12}, c^1_{21}, and c^1_{22} are examined [the equations from (1A) and (1B) elements of C_4R_2 and R_2C_4 do this], it will be found that there are only two independent equations, which may be written:

$$R_2 = \begin{array}{c} \begin{matrix} \frac{(x^2+y^2)}{\sqrt{2}} & z^2 & \frac{(x^2-y^2)}{\sqrt{2}} & xy & \frac{z(x+iy)}{\sqrt{2}} & \frac{z(x-iy)}{\sqrt{2}} \end{matrix} \\ \begin{bmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{-1}{2} & \cdot & \cdot & \cdot \\ \frac{1}{\sqrt{2}} & \cdot & \frac{1}{\sqrt{2}} & \cdot & \cdot & \cdot \\ \frac{-1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \cdot & \cdot & \cdot & \frac{-i}{\sqrt{2}} & \frac{1}{2} & \frac{1}{2} \\ \cdot & \cdot & \cdot & \frac{i}{\sqrt{2}} & \frac{1}{2} & \frac{1}{2} \end{bmatrix} \end{array}, \tag{5.6a}$$

$$R_4 = \begin{array}{c} \begin{matrix} \frac{(x^2+y^2)}{\sqrt{2}} & z^2 & \frac{(x^2-y^2)}{\sqrt{2}} & xy & \frac{z(x+iy)}{\sqrt{2}} & \frac{z(x-iy)}{\sqrt{2}} \end{matrix} \\ \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & -1 & & & \\ & & & -1 & & \\ & & & & i & \\ & & & & & -i \end{bmatrix} \end{array}, \tag{5.6b}$$

$$C_4 = \begin{bmatrix} c_{11}^1 & c_{12}^1 & & & & \\ c_{21}^1 & c_{22}^1 & & & & \\ & & c_{11}^{-1} & c_{12}^{-1} & & \\ & & c_{21}^{-1} & c_{22}^{-1} & & \\ & & & & c_{11}^{i} & \\ & & & & & c_{11}^{-i} \end{bmatrix}; \tag{5.6c}$$

$$C_4R_2 = \begin{bmatrix} \frac{c_{11}^1}{2} + \frac{c_{12}^1}{\sqrt{2}} & \frac{c_{11}^1}{\sqrt{2}} & -\frac{c_{11}^1}{2} + \frac{c_{12}^1}{\sqrt{2}} & . & . & . \\ \frac{c_{21}^1}{2} + \frac{c_{22}^1}{\sqrt{2}} & \frac{c_{21}^1}{\sqrt{2}} & -\frac{c_{21}^1}{2} + \frac{c_{22}^1}{\sqrt{2}} & . & . & . \\ -\frac{c_{11}^{-1}}{2} & \frac{c_{11}^{-1}}{\sqrt{2}} & \frac{c_{11}^{-1}}{2} & . & i\frac{c_{12}^{-1}}{\sqrt{2}} & -i\frac{c_{12}^{-1}}{\sqrt{2}} \\ -\frac{c_{21}^{-1}}{2} & \frac{c_{21}^{-1}}{\sqrt{2}} & \frac{c_{21}^{-1}}{2} & . & i\frac{c_{22}^{-1}}{\sqrt{2}} & -i\frac{c_{22}^{-1}}{\sqrt{2}} \\ . & . & . & -i\frac{c_{11}^{i}}{\sqrt{2}} & \frac{c_{11}^{i}}{2} & \frac{c_{11}^{i}}{2} \\ . & . & . & i\frac{c_{11}^{-i}}{\sqrt{2}} & \frac{c_{11}^{-i}}{2} & \frac{c_{11}^{-i}}{2} \end{bmatrix}, \tag{5.7a}$$

$$R_2C_4 = \begin{bmatrix} \frac{c_{11}^1}{2} + \frac{c_{21}^1}{\sqrt{2}} & \frac{c_{12}^1}{2} + \frac{c_{22}^1}{\sqrt{2}} & -\frac{c_{11}^{-1}}{2} & -\frac{c_{12}^{-1}}{2} & . & . \\ \frac{c_{11}^1}{\sqrt{2}} & \frac{c_{12}^1}{\sqrt{2}} & \frac{c_{11}^{-1}}{\sqrt{2}} & \frac{c_{12}^{-1}}{\sqrt{2}} & . & . \\ -\frac{c_{11}^1}{2} + \frac{c_{21}^1}{\sqrt{2}} & -\frac{c_{12}^1}{2} + \frac{c_{22}^1}{\sqrt{2}} & \frac{c_{11}^{-1}}{2} & \frac{c_{12}^{-1}}{2} & . & . \\ . & . & . & . & i\frac{c_{11}^{i}}{\sqrt{2}} & -i\frac{c_{11}^{-1}}{\sqrt{2}} \\ . & . & -i\frac{c_{21}^{-1}}{\sqrt{2}} & -i\frac{c_{22}^{-1}}{\sqrt{2}} & \frac{c_{11}^{i}}{2} & \frac{c_{11}^{-i}}{2} \\ . & . & i\frac{c_{21}^{-1}}{\sqrt{2}} & i\frac{c_{22}^{-1}}{\sqrt{2}} & \frac{c_{11}^{i}}{2} & \frac{c_{11}^{-i}}{2} \end{bmatrix}, \tag{5.7b}$$

$$c_{12}^1 = c_{21}^1, \tag{5.8}$$

$$c_{11}^1 = c_{12}^1/\sqrt{2} + c_{22}^1, \tag{5.9}$$

which shows that if C_{24} is the most general matrix that commutes with R_2 and R_4, then the submatrix of C_{24} which operates in the space spanned by $(x^2 + y^2)/\sqrt{2}$ and z^2 is an arbitrary linear combination of any two solutions of (5.8) and (5.9) since there are four unknowns and only two equations.

One possible solution is

$$c_{12}^1 = 1, \quad c_{21}^1 = 1, \quad c_{22}^1 = 0, \quad c_{11}^1 = c_{12}^1/\sqrt{2} = 1/\sqrt{2}, \tag{5.10}$$

i.e.,

$$C_4 = \begin{bmatrix} 1/\sqrt{2} & 1 \\ 1 & 0 \end{bmatrix}. \tag{5.11}$$

Section 2 shows that the two eigenvectors of this matrix belong to inequivalent representations

$$v_1 = \frac{\sqrt{2}}{\sqrt{3}}\left(\frac{x^2 + y^2}{\sqrt{2}}\right) + \frac{z^2}{\sqrt{3}} \tag{5.12}$$

and

$$v_2 = \left(\frac{x^2 + y^2}{\sqrt{2}\sqrt{3}}\right) - \frac{\sqrt{2}}{\sqrt{3}}(z^2). \tag{5.13}$$

Formation of the equations for the other submatrices of C_4^* show that v_1 belongs to a representation all by itself, but v_2 is a partner in a two-dimensional representation spanned by v_2 and $(x^2 - y^2)/\sqrt{2}$ because the condition (use row 3 col. 1) requires

$$-c_{11}^{-1}/2 = -c_{11}^1/2 + c_{21}^1/\sqrt{2}, \tag{5.14}$$

which determines c_{11}^{-1} once c_{11}^1 and c_{21}^1 are known.

In fact, c_{11}^{-1} is an eigenvalue of 5.109.

Similarly $xy/\sqrt{3}$, $z(x + iy)/\sqrt{3}$, and $z(x - iy)/\sqrt{3}$ span a 3-dimensional irreducible representation.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Diffraction of Plane Acoustic Waves and Pulses as a Singular Perturbation Problem

EDWARD Y. HARPER*
Lockheed Palo Alto Research Laboratory, Palo Alto, California

(Received 31 January 1969)

The diffraction of plane waves and pulses by cylindrical cavities is studied as a singular perturbation problem for long waves and broad pulses. The solution, which is obtained to a given order of approximation by the method of matched asymptotic expansions, is applicable to arbitrary cavity shapes and, in the case of pulse diffraction, incident profiles of arbitrary form.

I. INTRODUCTION

Investigations relative to the scattering of weak sound pulses by objects of various shapes and compositions have aimed, in particular, at finding the level of disturbance immediately behind the outgoing wave front, that is, for "short times" after the arrival of the front at a given location.[1–3] A "long time" solution, applicable well to the rear of the expanding front, has been obtained by Chen[4] for plane pulses incident upon a rigid circular cylinder and a hollow circular inclusion or cavity. In the latter cases the analysis, based on a Laplace transform with respect to the time variable and a small argument approximation for the appropriate mode expansion, reveals distinctive limiting responses to an incoming unit pressure front (Heaviside step function): specifically, for the rigid cylinder a steady state is approached with a pressure distribution that is everywhere equal to unity, whereas, for the cavity, the pressure approaches zero in an inverse logarithmic fashion at a given position. In contrast to the implied tendency of the cavity to depress the pressure level, there is a logarithmic growth of the pressure with distance from the cavity for large fixed values of the time.

The solution obtained by Chen bears a considerable resemblance to that which obtains in the Stokes approximation for the plane flow of an incompressible viscous fluid past a cylinder at low Reynolds numbers. In the hydrodynamic problem Stokes was able to meet the boundary conditions on the cylinder, but not at

* Now at the Bell Telephone Laboratory.

[1] F. G. Friedlander, *Sound Pulses* (Cambridge University Press, Cambridge, England, 1958).

[2] S. K. Mishra, Proc. Cambridge Phil. Soc. **60**, 295 (1964).

[3] H. Uberall, R. Dolittle, and J. McNicholas, J. Acoust. Soc. Am. **39**, 564 (1966).

[4] Y. M. Chen, Intern. J. Eng. Sci. **2**, 417 (1964).

$$c_{12}^1 = c_{21}^1, \tag{5.8}$$

$$c_{11}^1 = c_{12}^1/\sqrt{2} + c_{22}^1, \tag{5.9}$$

which shows that if C_{24} is the most general matrix that commutes with R_2 and R_4, then the submatrix of C_{24} which operates in the space spanned by $(x^2 + y^2)/\sqrt{2}$ and z^2 is an arbitrary linear combination of any two solutions of (5.8) and (5.9) since there are four unknowns and only two equations.

One possible solution is

$$c_{12}^1 = 1, \quad c_{21}^1 = 1, \quad c_{22}^1 = 0, \quad c_{11}^1 = c_{12}^1/\sqrt{2} = 1/\sqrt{2}, \tag{5.10}$$

i.e.,

$$C_4 = \begin{bmatrix} 1/\sqrt{2} & 1 \\ 1 & 0 \end{bmatrix}. \tag{5.11}$$

Section 2 shows that the two eigenvectors of this matrix belong to inequivalent representations

$$v_1 = \frac{\sqrt{2}}{\sqrt{3}}\left(\frac{x^2 + y^2}{\sqrt{2}}\right) + \frac{z^2}{\sqrt{3}} \tag{5.12}$$

and

$$v_2 = \left(\frac{x^2 + y^2}{\sqrt{2}\sqrt{3}}\right) - \frac{\sqrt{2}}{\sqrt{3}}(z^2). \tag{5.13}$$

Formation of the equations for the other submatrices of C_4^* show that v_1 belongs to a representation all by itself, but v_2 is a partner in a two-dimensional representation spanned by v_2 and $(x^2 - y^2)/\sqrt{2}$ because the condition (use row 3 col. 1) requires

$$-c_{11}^{-1}/2 = -c_{11}^1/2 + c_{21}^1/\sqrt{2}, \tag{5.14}$$

which determines c_{11}^{-1} once c_{11}^1 and c_{21}^1 are known.

In fact, c_{11}^{-1} is an eigenvalue of 5.109.

Similarly $xy/\sqrt{3}$, $z(x + iy)/\sqrt{3}$, and $z(x - iy)/\sqrt{3}$ span a 3-dimensional irreducible representation.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Diffraction of Plane Acoustic Waves and Pulses as a Singular Perturbation Problem

EDWARD Y. HARPER*
Lockheed Palo Alto Research Laboratory, Palo Alto, California

(Received 31 January 1969)

The diffraction of plane waves and pulses by cylindrical cavities is studied as a singular perturbation problem for long waves and broad pulses. The solution, which is obtained to a given order of approximation by the method of matched asymptotic expansions, is applicable to arbitrary cavity shapes and, in the case of pulse diffraction, incident profiles of arbitrary form.

I. INTRODUCTION

Investigations relative to the scattering of weak sound pulses by objects of various shapes and compositions have aimed, in particular, at finding the level of disturbance immediately behind the outgoing wave front, that is, for "short times" after the arrival of the front at a given location.[1–3] A "long time" solution, applicable well to the rear of the expanding front, has been obtained by Chen[4] for plane pulses incident upon a rigid circular cylinder and a hollow circular inclusion or cavity. In the latter cases the analysis, based on a Laplace transform with respect to the time variable and a small argument approximation for the appropriate mode expansion, reveals distinctive limiting responses to an incoming unit pressure front (Heaviside step function): specifically, for the rigid cylinder a steady state is approached with a pressure distribution that is everywhere equal to unity, whereas, for the cavity, the pressure approaches zero in an inverse logarithmic fashion at a given position. In contrast to the implied tendency of the cavity to depress the pressure level, there is a logarithmic growth of the pressure with distance from the cavity for large fixed values of the time.

The solution obtained by Chen bears a considerable resemblance to that which obtains in the Stokes approximation for the plane flow of an incompressible viscous fluid past a cylinder at low Reynolds numbers. In the hydrodynamic problem Stokes was able to meet the boundary conditions on the cylinder, but not at

* Now at the Bell Telephone Laboratory.

[1] F. G. Friedlander, *Sound Pulses* (Cambridge University Press, Cambridge, England, 1958).

[2] S. K. Mishra, Proc. Cambridge Phil. Soc. **60**, 295 (1964).

[3] H. Uberall, R. Dolittle, and J. McNicholas, J. Acoust. Soc. Am. **39**, 564 (1966).

[4] Y. M. Chen, Intern. J. Eng. Sci. **2**, 417 (1964).

large distances away therefrom; his interpretation of the result led to erroneous conclusions regarding the physical behavior of the flow field and the cylinder drag. The Stokes problem has been resolved by contemporary investigators in terms of singular perturbation theory.[5] Within the framework of this theory, the Stokes solution forms the basis of an inner expansion valid near the body while an outer expansion, valid far from the body, is required in order to complete the description everywhere. The purpose of this paper is to apply a similar technique in the context of acoustical scattering so as to obtain a meaningful physical description of the field everywhere. It will be shown that the leading term of Chen's solution is valid in the neighborhood of the cylinder, that is, for distances from the cylinder boundary which are comparable to or less than its radius, but ceases to apply at distances much longer than the cylinder radius. Our analysis makes it apparent that a small cavity has only a local effect on a relatively broad pressure pulse, and details this effect to a second order of approximation. Apart from the particular application which forms the substance of this paper, it is hoped that the technique of inner and outer expansions, elaborated for the most part in problems of fluid mechanics,[6] will recommend itself for the analysis of wave propagation and scattering. In order to illustrate the technique and prepare the way for the consideration of pulse diffraction, a detailed mathematical analysis is initially developed for the scattering of plane harmonic waves by a circular cavity.

II. INNER AND OUTER EXPANSIONS

Scattering problems involving time-periodic waves feature a dimensionless parameter given by the ratio of obstacle size and wavelength. For nonperiodic excitations the breadth of the incident pulse takes over the role of the wavelength in the analogous parameter, or else the latter contains a characteristic length defined by the product of wave speed and time when the pulse has unlimited extension. A complicating aspect of these problems is that a single asymptotic expansion in terms of such a parameter may not be uniformly valid in space. We shall attempt to construct a solution to the pulse problem in terms of inner and outer expansions for small values of the ratio of cylinder diameter to pulse length; this choice for the perturbation parameter is motivated by our intention to apply the explicit solution to the plane-wave scattering problem at long wavelengths.

The ratio of cylinder diameter to pulse length (or wavelength) may approach zero in different ways corresponding to two distinct physical problems. In one limit the obstacle contracts to a point while the wave or pulse length remains fixed and in the other limit the wave or pulse grows in length without alteration of the body size. In such circumstances two asymptotic expansions may be required: an inner expansion which meets boundary conditions on the cylinder but not at great distances, and an outer expansion which is valid far from the cylinder but fails to meet boundary conditions on its surface. These two expansions share a region of common validity and may be matched to a given order in the perturbation parameter. The matching permits a determination of both the form and coefficients of the asymptotic sequences and, moreover, rules out certain eigensolutions in both expansions. For the case of diffraction by a circular cavity, the exact solution is known and thus, in principle, the inner and outer expansions may be obtained directly and their overlap demonstrated by matching. However, it is instructive to develop these expansions without resorting to the exact solution in order to guide the analysis for other cavity shapes. In addition, matching affords an alternative to a formal expansion of the exact solution if such an expansion proves difficult.

III. PLANE-WAVE SCATTERING BY A CIRCULAR CAVITY AT LONG WAVELENGTHS

The pressure fluctuation $\Psi(\mathbf{r}, t)$ satisfies a homogeneous wave equation in source free regions, with the two-dimensional version

$$\nabla_{r,\theta}^2 \Psi = \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\right)\Psi = \frac{1}{c^2}\frac{\partial^2 \Psi}{\partial t^2}, \quad (1)$$

where r, θ designate polar coordinates, t is the time, and c denotes the sound speed. In terms of a dimensionless time, $T = kct$, simply periodic pressure fluctuations are represented by

$$\Psi = \mathrm{Re}\ \psi(\mathbf{r})e^{-iT}, \quad (2a)$$

where

$$\nabla_{r,\theta}^2 \psi + k^2 \psi = 0 \quad (2b)$$

and k designates the wave number. For an incident plane wave

$$\psi_{\mathrm{inc}} = e^{ikr\cos\theta}, \quad (3a)$$

the outward-going or scattered wave which conforms with Eq. (3a) is described by a Fourier expansion in

[5] S. Kaplun, J. Ratl. Mech. Anal. 6, 595 (1957).
[6] M. D. Van Dyke, *Perturbation Methods in Fluid Mechanics* (Academic Press Inc., New York, 1964).

terms of Hankel functions of the first kind

$$\psi_{sc} = \sum_{-\infty}^{\infty} A_n H_n^{(1)}(kr) \cos n\theta, \tag{3b}$$

and the boundary condition appropriate to a cavity takes the form

$$\psi(a, \theta) = \psi_{inc}(a, \theta) + \psi_{sc}(a, \theta) = 0. \tag{3c}$$

We shall consider the circumstance in which the wavelength is large compared with the cavity radius, whence

$$\epsilon = ka \ll 1 \tag{4}$$

is a small parameter, and observe that the limit $\epsilon \to 0$ is realized by the alternatives

$$k \to 0, \quad a \text{ fixed}, \tag{5a}$$

$$a \to 0, \quad k \text{ fixed}. \tag{5b}$$

The former limit corresponds to an inner problem where the appropriate length scale is a, and the latter corresponds to an outer problem where the appropriate length scale is k^{-1}.

Inner Problem: $k \to 0$, a fixed

We define an inner variable

$$\rho = r/a \tag{6}$$

in terms of which the differential equation for the scattered wave and the boundary condition take the forms

$$\nabla^2_{\rho,\theta}\psi_{sc} + \epsilon^2\psi_{sc} = 0, \tag{7a}$$

$$\psi_{sc}(1, \theta) = -\psi_{inc}(1, \theta). \tag{7b}$$

If we expand ψ_{inc} for small ϵ,

$$\psi_{inc} = e^{i\epsilon\rho\cos\theta} \sim 1 + O(\epsilon), \tag{8}$$

and discard terms of $O(\epsilon)$, but not of lower order, the corresponding specification for ψ_{sc} involves the Laplace differential equation

$$\nabla^2_{\rho,\theta}\psi_{sc} = 0 \tag{9a}$$

and the boundary condition

$$\psi_{sc}(1, \theta) = -1. \tag{9b}$$

The general solution to Eqs. (9a) and (9b) may be written as

$$\psi_{sc} = -1 + \Delta_0(\epsilon) \ln \rho + \sum_{1}^{\infty} \Delta_m(\epsilon)[\rho^m - \rho^{-m}] \cos m\theta, \tag{10}$$

where the sequence $\Delta_m(\epsilon)$, $m = 0, 1, 2, \cdots$, is to be determined by matching with an outer expansion for ψ. It will be shown that, to the present order of approximation, only $\Delta_0(\epsilon)$ is different from zero, for the infinite series in (10) cannot be matched to an outer expansion for ψ with nonzero values of $\Delta_m(\epsilon)$, $m \geq 1$. Thus, we write the inner expansion to $O(\Delta_0)$ as

$$\psi_{inner} \sim \Delta_0(\epsilon) \ln \rho \tag{11}$$

and turn our attention to the outer expansion.

Outer Problem: $a \to 0$, k fixed

We define an outer coordinate

$$\tilde{\rho} = kr, \tag{12}$$

in terms of which the differential equation (2b) assumes the form

$$\nabla^2_{\tilde{\rho},\theta}\psi + \psi = 0. \tag{13}$$

A particular solution of Eq. (13),

$$\psi \sim e^{i\tilde{\rho}\cos\theta}, \tag{14}$$

which represents the incident or undiffracted wave, constitutes the leading term of the outer expansion.

For the next term of the outer expansion the body may be characterized as a line source, and thus

$$\psi \sim e^{i\tilde{\rho}\cos\theta} + A_0(\epsilon)H_0^{(1)}(\tilde{\rho}), \tag{15}$$

where $A_0(\epsilon)$, the source strength, is to be determined by matching with the inner expansion. Further terms of the outer expansion, with the collective representation

$$\sum_{1}^{\infty} A_n(\epsilon)H_n^{(1)}(\tilde{\rho}) \cos n\theta, \tag{16}$$

may be regarded as higher order inasmuch as the leading term of the inner expansion evidences no angular dependence.

Matching

The matching is carried out in accord with a rule set forth by Van Dyke,[6] according to which the inner expansion (to order α) of the outer expansion (to order β) is equivalent to the outer expansion (to order β) of the inner expansion (to order α). We first determine $\Delta_0(\epsilon)$ by matching the leading terms of the inner and outer expansions. From Eqs. (11) we have, for the inner expansion to $O(\Delta)$,

$$\psi \sim \Delta_0(\epsilon) \ln \rho. \tag{17a}$$

Rewritten in outer variables, we have

$$\psi \sim \Delta_0(\epsilon)[\ln (\epsilon)^{-1} + \ln \tilde{\rho}]. \tag{17b}$$

For the outer expansion to $O(\Delta_0 \ln (\epsilon)^{-1})$ of the inner expansion to $O(\Delta_0)$, we have

$$\psi \sim \Delta_0(\epsilon) \ln (\epsilon)^{-1}. \tag{17c}$$

From Eq. (14) we have, for the outer expansion to $O(1)$,

$$\psi \sim e^{i\tilde{\rho}\cos\theta}. \tag{17d}$$

Written in inner variables, we have

$$\psi \sim e^{i\epsilon\rho\cos\theta}. \tag{17e}$$

For the inner expansion to $O(\Delta_0)$ of the outer expansion to $O(1)$, we have

$$\psi \sim 1. \tag{17f}$$

The equivalence of (17c) and (17f) yields

$$\Delta_0(\epsilon) = [1/\ln(\epsilon)^{-1}], \tag{18}$$

and this determination ensures that the matching has been carried out in accord with the rule given.

In order to specify the source strength $A_0(\epsilon)$ in the second term of the outer expansion, we match the two-term outer expansion with the one-term inner expansion. From Eq. (15), as the outer expansion to $O(A_0)$, we have

$$\psi \sim e^{i\tilde{\rho}\cos\theta} + A_0(\epsilon)H_0^{(1)}(\tilde{\rho}). \tag{19a}$$

Written in inner variables, we have

$$\psi \sim e^{i\epsilon\rho\cos\theta} + A_0(\epsilon)H_0^{(1)}(\epsilon\rho). \tag{19b}$$

After expansion for small ϵ, we have

$$\psi \sim 1 + A_0(\epsilon)i\frac{2}{\pi}\left[\ln\epsilon + \ln\frac{\rho}{2} - i\frac{\pi}{2} + C\right], \tag{19c}$$

where $C = 0.577$ is Euler's constant, and thus, as the inner expansion to $O(A_0\ln\epsilon)$ of the outer expansion to $O(A_0)$, we have

$$\psi \sim 1 + A_0(\epsilon)i(2/\pi)\ln\epsilon. \tag{19d}$$

The determination of $\Delta_0(\epsilon)$, Eq. (18), shows that the outer expansion to $O(1/\ln\epsilon)$ of the inner expansion to $O(1)$ is

$$\psi = 0. \tag{19e}$$

Accordingly, the equivalence of (19d) and (19e) yields

$$A_0(\epsilon) = -\tfrac{1}{2}i\pi[1/\ln(\epsilon)^{-1}]. \tag{20}$$

A refinement of the inner expansion, Eq. (17a), which is to say a determination of $\Delta_0(\epsilon)$ that goes beyond Eq. (18) through the inclusion of terms of $O(1/\ln^P\epsilon)$, $P > 1$, can be initiated with the representation

$$\psi \sim [1/(\ln(\epsilon)^{-1} + \kappa)]\ln\rho, \tag{21}$$

where κ is a constant. On expanding the coefficient of $\ln\rho$ in Eq. (21), for the inner expansion to $O(1/\ln^2\epsilon)$, we have

$$\psi \sim \frac{\ln\rho}{\ln(\epsilon)^{-1}}\left[1 - \frac{\kappa}{\ln(\epsilon)^{-1}}\right]. \tag{22a}$$

Written in outer variables, we have

$$\psi \sim \left[1 + \frac{\ln\tilde{\rho}}{\ln(\epsilon)^{-1}}\right]\left[1 - \frac{\kappa}{\ln(\epsilon)^{-1}}\right]. \tag{22b}$$

Expanded to $O(1/\ln\epsilon)$, we have

$$\psi \sim 1 + \frac{1}{\ln(\epsilon)^{-1}}[\ln\tilde{\rho} - \kappa] = \frac{1}{\ln(\epsilon)^{-1}}[\ln\tilde{\rho} - \kappa]. \tag{22c}$$

In order to determine κ we arrange for the equivalence of (22c) with the inner expansion to $O(1/\ln^2\epsilon)$ of the outer expansion to $O(1/\ln\epsilon)$, namely,

$$\psi \sim \frac{1}{\ln(\epsilon)^{-1}}[\ln\rho + \ln\tfrac{1}{2} + C - \tfrac{1}{2}i\pi], \tag{22d}$$

and the outcome is that

$$\kappa = \tfrac{1}{2}i\pi - [C + \ln\tfrac{1}{2}] = 0.116 + \tfrac{1}{2}i\pi. \tag{23}$$

The corresponding refinement of the source strength A_0 in the outer expansion is achieved by matching the outer expansion to $O(1/\ln^2\epsilon)$ of inner expansion to $O(1/\ln^2\epsilon)$:

$$\frac{\ln\rho}{\ln(\epsilon)^{-1}}\left[1 - \frac{\tfrac{1}{2}i\pi + 0.116}{\ln(\epsilon)^{-1}}\right] \tag{24a}$$

with the inner expansion to $O(A_0)$ of outer expansion to $O(A_0)$:

$$\psi \sim 1 + A_0(\epsilon)i(2/\pi)[\ln\epsilon + \ln\rho - \tfrac{1}{2}i\pi - 0.116]. \tag{24b}$$

The result is

$$A_0 = -\frac{\tfrac{1}{2}i\pi}{\ln(\epsilon)^{-1}}\left[1 - \frac{\tfrac{1}{2}i\pi + 0.116}{\ln(\epsilon)^{-1}}\right] \tag{25}$$

and, consequently, we find, for the outer expansion to $O(1/\ln^2\epsilon)$,

$$\psi_{\text{outer}} \sim e^{i\tilde{\rho}\cos\theta} - i\frac{\pi}{2}\frac{1}{\ln(\epsilon)^{-1}}\left[1 - \frac{\tfrac{1}{2}i\pi + 0.116}{\ln(\epsilon)^{-1}}\right]H_0^{(1)}(\tilde{\rho}). \tag{26a}$$

The foregoing outer expansion and the inner expansion based on the determination Eq. (21) for κ,

$$\psi_{\text{inner}} \sim \frac{\ln\rho}{\ln(\epsilon)^{-1} + \tfrac{1}{2}i\pi + 0.116}, \tag{26b}$$

are precisely reproduced when the exact solution of the problem

$$\psi = e^{ikr\cos\theta} - \sum_{-\infty}^{\infty} i^n e^{in\theta}\frac{J_n(ka)}{H_n^{(1)}(ka)}H_n^{(1)}(kr) \tag{27}$$

is written in the appropriate outer or inner variables and expanded for small ϵ to $O(1/\ln^2\epsilon)$.

That inner and outer expansions are jointly involved in the plane-wave diffraction problem and may be characterized without reference to an exact solution is of particular relevance to the analysis of the corresponding diffraction problem for other cavity shapes.

IV. SCATTERING OF BROAD PULSES BY A CIRCULAR CAVITY

We begin by introducing a new outer length $c\tau$, where τ is a characteristic time associated with the incident pulse P_{inc}. In order to compare our results with those of Chen, we will consider a rectangular profile, traveling in the positive x direction and of duration 2τ at any fixed point, given by

$$P_{\text{inc}}\left[\frac{1}{\tau}\left(t-\frac{x}{c}\right)\right] = H\left[\frac{1}{\tau}\left(t-\frac{x}{c}\right)+1\right] - H\left[\frac{1}{\tau}\left(t-\frac{x}{c}\right)-1\right], \quad (28a)$$

where H is the Heaviside step function. As a representative of smooth incident pulses with unlimited extension we choose the form

$$P_{\text{inc}}\left[\frac{1}{\tau}\left(t-\frac{x}{c}\right)\right] = \left\{1+\left[\frac{1}{c}\left(t-\frac{x}{c}\right)\right]^2\right\}^{-1}. \quad (28b)$$

The object of our analysis is to obtain a uniformly valid asymptotic description for the scattering of such pulses by a circular cavity of radius a when

$$R = a/c\tau \ll 1. \quad (29)$$

In order to link the solutions which correspond, on the one hand, to small values of the parameter R and, on the other hand, to large values of the time (Chen), let us consider the incident rectangular profile: in outer variables, where the coordinate $\tilde{\rho}$ is defined by

$$\tilde{\rho} = r/c\tau, \quad (30)$$

the pulse is centered over the cylinder at the time $t = 0$ and extends over the interval $|x| \leq 1$, which is large compared with the cylinder radius R. The location of the front with respect to the surface of the cylinder may be adjusted by varying the value of R and in this sense R is "timelike." It should be noted that in the case of the rectangular pulse the choice $t = 0$ can be made without loss of generality. The explicit relation between R and Chen's time T_c may then be written as

$$T_c = ct_c/a = 1/R + 1, \quad (31)$$

where $t_c = 0$ corresponds to the moment an incident Heaviside step profile first contacts the surface of the cavity. Because the relief portion of the rectangular profile has not reached the cavity at $t = 0$, the diffraction pattern at small values of R is identical with that envisaged by Chen for a step profile at large values of t_c. In the case of other primary wave forms, such as the smooth profile of Eq. (28b), the time must appear as a parameter of the scattering problem and may be rendered dimensionless in accordance with the definition

$$T_0 = t/\tau. \quad (32)$$

It should be noted that the time for passage of the incident profile over the cavity, namely a/c, is much smaller than τ and does not provide an appropriate reference scale for a "long-time" expansion.

The Exact Solution

The complete solution may be written as the sum of an incident plane pulse,

$$P_{\text{inc}}[T_0 - x/c\tau], \quad (33)$$

together with a scattered pulse,

$$P_{\text{sc}}(r, \theta, T_0) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega_0)e^{-iT_0\omega_0} \times \sum_{-\infty}^{\infty} i^n e^{in\theta}\frac{J_n(\omega_0 R)}{H_n^{(1)}(\omega_0 R)} H_n^{(1)}\left(\frac{\omega_0}{c\tau}r\right) d\omega_0, \quad (34a)$$

where

$$x = r\cos\theta \quad \text{and} \quad \omega_0 = kc\tau \quad (34b)$$

and where $F(\omega_0)$ is the Fourier transform of the incident pulse

$$F(\omega_0) = \int_{-\infty}^{\infty} P_{\text{inc}}(T_0)e^{i\omega_0 T_0}\, dT_0. \quad (34c)$$

Since

$$P_{\text{inc}}(T_0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega_0)e^{-iT_0\omega_0}\, d\omega_0 \quad (35)$$

is real, we conclude that $F(\omega_0)$ has the Hermitian property

$$F(\omega_0) = F^*(\omega_0), \quad (36)$$

where the asterisk denotes the complex conjugate. The latter property is also manifest by the normal mode series in Eq. (34a) and consequently the exact solution may be displayed in the form

$$P = P_{\text{inc}}\left(T_0 - \frac{r\cos\theta}{c\tau}\right) - \text{Re}\,\frac{1}{\pi}\int_0^{\infty} F(\omega_0) \times e^{-iT_0\omega_0}\sum i^n e^{in\theta}\frac{J_n(\omega_0 R)}{H_n^{(1)}(\omega_0 R)} H_n^{(1)}\left(\frac{\omega_0}{c\tau}r\right) d\omega_0. \quad (37)$$

We begin our determination of a uniformly valid asymptotic description for the problem of pulse diffraction by a circular cavity, with a discussion of the formal expansion of the exact solution.

The Inner Expansion: $R \to 0$, $\rho = r/a$ fixed

In terms of inner variables ρ, θ, the representation Eq. (37) is

$$P_{\text{inner}} = P_{\text{inc}}(T_0 - R\rho\cos\theta) - \operatorname{Re}\frac{1}{\pi}\int_0^\infty F(\omega_0) \times e^{-iT_0\omega_0}\sum i^n e^{in\theta}\frac{J_n(\omega_0 R)}{H_n^{(1)}(\omega_0 R)} H_n^{(1)}(\rho\omega_0 R)\, d\omega_0. \tag{38}$$

A small-argument approximation

$$\omega_0 R = o(1) \tag{39a}$$

leads to the asymptotic form

$$P_{\text{inner}} \sim \Delta(T_0; R)\ln\rho, \tag{39b}$$

where

$$\Delta(T_0; R) = \operatorname{Re}\lim_{\omega\to\infty}\frac{1}{\pi} \times\int_0^\omega \frac{F(\omega_0)e^{-iT_0\omega_0}}{[\ln(\omega_0 R)^{-1} - \ln\tfrac{1}{2} - C + \tfrac{1}{2}i\pi]}\, d\omega_0 \tag{39c}$$

and where the designation of the upper limit ω warrants further discussion. Since $\rho = O(1)$ in the inner region, the approximation (39a) requires that $\omega = o(1/R)$. Inspection of Eq. (26b) and recognition of the identity

$$\epsilon = \omega_0 R \tag{39d}$$

reveals that the coefficient $\Delta(T_0; R)$ is a Fourier synthesis of the scattered pulse which employs low frequencies, that is, wavelengths which are long in comparison with the cylinder. Therefore, we employ the physically meaningful upper limit

$$\omega = O(1/R^n), \quad 0 < n < 1, \tag{39e}$$

which is consistent with the approximations (39a). If we assume that $F(\omega_0)$ is integrable at the lower limit $\omega_0 = 0$, we may expand Eq. (39c) further as

$$\Delta(T_0; R) \sim \frac{\operatorname{Re}}{\ln R^{-1}}\left\{\int_0^{R^{-n}} F(\omega_0)\, d\omega_0 + \frac{1}{\ln R^{-1}}\frac{1}{\pi} \times\int_0^{R^{-n}} F(\omega_0)\left[\ln\frac{\omega_0}{2} + C - i\frac{\pi}{2}\right] d\omega_0\right\}, \tag{40}$$

where the error arising from the expansion in the interval $0 \le \omega_0 \le R$ is of $O(R/\ln R)$.

The functions $F(\omega_0)$ for the rectangular wave, Eq. (28a), and the smooth wave, Eq. (28b), are

$$2(\sin\omega_0)/\omega_0 \quad \text{and} \quad \pi e^{-|\omega_0|}, \tag{41a}$$

respectively. The results obtained by substituting these functions into the first integral of Eq. (40),

$$1 + O(R^n) \quad \text{and} \quad \frac{1}{1+T_0^2} + O(e^{-R^{-n}}), \tag{41b}$$

indicate that the leading term of the inner expansion is proportional to the amplitude of the incident pulse at $x = 0$. This conclusion may be substantiated by observing that the leading term of the outer expansion is just the incident pulse

$$P_{\text{outer}} \sim P_{\text{inc}}[T_0 - \tilde{\rho}\cos\theta] \tag{42a}$$

and this has nearly the constant value

$$\sim P_{\text{inc}}(T_0) \tag{42b}$$

near the cavity. The necessary compatibility of (39b) and (42b), based on the matching rule, reveals that in the first approximation

$$\Delta(T_0; R) = [P_{\text{inc}}(T_0)/\ln(R)^{-1}]. \tag{43}$$

Therefore, the asymptotic representation of the inner expansion is

$$P_{\text{inner}} \sim [P_{\text{inc}}(T_0)/\ln(R)^{-1}]\ln\rho. \tag{44}$$

In the special case of the rectangular pulse,

$$P_{\text{inc}}(T_0 = 0) = 1,$$

we recover Chen's leading term from Eq. (44) after eliminating R in favor of T_c by means of Eq. (31). Our result is more general, however, in that it reveals a level of excitation near the cavity which is proportional to the local amplitude of an incident pulse of arbitrary shape.

A refinement of the inner expansion to $O(1/\ln^2\epsilon)$ is now initiated with the representation

$$P_{\text{inner}} \sim \frac{P_{\text{inc}}(T_0)}{\ln(R)^{-1} + \kappa(T_0)}\ln\rho \sim \frac{P_{\text{inc}}(T_0)}{\ln(R)^{-1}}\left[1 - \frac{\kappa(T_0)}{\ln(R)^{-1}}\right]\ln\rho, \tag{45a}$$

whence, from Eq. (40), we have

$$\kappa(T_0) = \frac{\operatorname{Re}}{P_{\text{inc}}(T_0)}\lim_{R\to 0}\frac{1}{\pi}\int_0^{R^{-n}} F(\omega_0) \times\left[\ln\frac{\omega_0}{2} + C - i\frac{\pi}{2}\right] d\omega_0. \tag{45b}$$

The formulation (45b) for $\kappa(T_0)$ is based on a direct expansion of the exact solution in inner variables.

Another formulation for $\kappa(T_0)$, based on the requisite condition for matching with an asymptotic expansion which is valid in the outer region, will now be developed. The advantage of this approach has been displayed in establishing a generalization to arbitrary pulse shape for the leading term. A further advantage will accrue should a ready estimate of the integral in (45b) prove difficult. In addition, the generalization of the solution to arbitrary cavity shape is based on a formulation in terms of matched asymptotic expansions.

Following the expansion procedure detailed in obtaining Eq. (22c), we write Eq. (45a), for large values of ρ, as

$$P_{\text{inner}} \sim \frac{P_{\text{inc}}(T_0)}{\ln (R)^{-1}} [\ln \rho - \kappa(T_0)] \tag{46}$$

and note that $\kappa(T_0)$ may be obtained by matching (46) with the outer expansion to $O(1/\ln R)$.

The Outer Expansion: $R \to 0$, $\tilde{\rho} = r/c\tau$ fixed

The exact solution in outer variables is

$$P_{\text{outer}} = P_{\text{inc}}(T_0 - \tilde{\rho}\cos\theta) - \operatorname{Re}\frac{1}{\pi}\int_0^\infty F(\omega_0) \times e^{-iT_0\omega_0}\sum i^n e^{in\theta}\frac{J_n(R\omega_0)}{H_n^{(1)}(R\omega_0)} H_n^{(1)}(\tilde{\rho}\omega_0)\, d\omega_0. \tag{47}$$

The small-argument approximation (39a) yields the asymptotic form

$$\sim P_{\text{inc}}(T_0 - \tilde{\rho}\cos\theta) - \operatorname{Re}\frac{1}{\pi}\int_0^{R^{-n}} F(\omega_0) \times e^{-iT_0\omega_0}\left(i\frac{\pi}{2}\frac{1}{\ln \omega_0 R}\right) H_0^{(1)}(\tilde{\rho}\omega_0)\, d\omega_0, \tag{48}$$

where the upper limit is self-consistent and where the coefficient of the Hankel function is the long-wavelength source strength A_0 of Eq. (20) with the change of variable (39d) and the restriction $\epsilon = o(1)$. We rewrite (48) to $O(1/\ln R)$ as

$$P_{\text{outer}} \sim P_{\text{inc}}(T_0 - \tilde{\rho}\cos\theta) - \frac{1}{\ln (R)^{-1}}\operatorname{Re}\frac{i}{2} \times \int_0^{R^{-n}} F(\omega_0) e^{-iT_0\omega_0} H_0^{(1)}(\tilde{\rho}\omega_0)\, d\omega_0, \tag{49}$$

which, when expanded for small values of $\tilde{\rho}$, must match Eq. (46), thereby determining $\kappa(T_0)$. It should be noted that an evaluation of the integral in Eq. (49) is, in general, less difficult than the quadrature required in Eq. (45b) which involves $\ln \omega_0$.

Smooth Pulse with Unlimited Extension

We proceed to find the parameter $\kappa(T_0)$ of Eq. (45a) for the case of the incident pulse shape described by Eq. (28b). A direct evaluation of the integral in Eq. (45b) leads to the result

$$\kappa(T_0) = \ln 2 + \tfrac{1}{2}\pi T_0 + \ln (1 + T_0^2)^{\frac{1}{2}} + T_0 \tan^{-1} T_0, \tag{50}$$

where terms of $O(e^{-R^{-n}} \ln R)$ arising from the integration have been dropped in the limiting process.

The alternative matching procedure requires an evaluation of the integral in Eq. (49):

$$\operatorname{Re} i\frac{\pi}{2}\int_0^{R^{-n}} e^{-(1+iT_0)\omega_0} H_0^{(1)}(\omega_0\tilde{\rho})\, d\omega_0 = \operatorname{Re}\frac{1}{[(1 + iT_0)^2 + \tilde{\rho}^2]^{\frac{1}{2}}} \times \left\{\ln \frac{1 + iT_0 + [(1 + iT_0)^2 + \tilde{\rho}^2]^{\frac{1}{2}}}{\tilde{\rho}} + i\frac{\pi}{2}\right\} + o(e^{-R^{-n}}). \tag{51}$$

After substituting from this result into Eq. (49) and rewriting in inner variables, we obtain the expansion

$$P \sim [(1 + T_0^2)^{-1}/\ln (R)^{-1}]\left[\ln \rho - \left(\ln 2 + \frac{\pi}{2} T_0 + \ln (1 + T_0^2)^{\frac{1}{2}} + T_0 \tan^{-1} T_0\right)\right], \tag{52}$$

which, when matched with Eq. (46), reproduces the value for $\kappa(T_0)$ given by Eq. (50).

Rectangular Pulse

A direct evaluation of the integral in Eq. (45b) for the case of the incident rectangular profile (28a) leads to the result

$$\kappa(T_0) = \ln 2, \tag{53}$$

where terms of $O(R^n \ln R)$ have been dropped in the limit.

The indirect matching procedure, which involves the integral

$$\int_0^{R^{-n}} \frac{\sin \omega_0}{\omega_0} y_0^{(1)}(\tilde{\rho}\omega_0)\, d\omega_0 = \ln \frac{1 - (1 - \tilde{\rho}^2)^{\frac{1}{2}}}{\tilde{\rho}} + o(R^n), \tag{54}$$

leads to an outer expansion of the form

$$P_{\text{outer}} \sim \{H[1 - \tilde{\rho}\cos\theta] - H[-1 - \tilde{\rho}\cos\theta]\} + \frac{1}{\ln (R)^{-1}} \ln \frac{1 - (1 - \tilde{\rho}^2)^{\frac{1}{2}}}{\tilde{\rho}}. \tag{55}$$

The expression which arises from rewriting Eq. (55)

in inner variables and expanding for small R,

$$\sim [1/\ln (R)^{-1}][\ln \rho - \ln 2], \tag{56}$$

may be matched with Eq. (46) to obtain the previous result (53).

V. COMPOSITE EXPANSION

For the purpose of clarity we shall discuss the specific result obtained for the diffraction of a broad rectangular pulse, traveling in the positive x direction, by a small circular cavity. The leading term of the outer expansion is the primary or incident pulse, which means that at great distances from the cavity the profile is unaffected by the encounter. However, in the neighborhood of the cavity, the amplitude of the total pulse is pulled down to a value consistent with the boundary condition on the cylinder. It is quite easy and instructive to form a single expansion which is uniformly valid to a given order. Such composite formulations[6] are not unique but do have the accuracy of the constituent inner and outer expansions in their regions of validity. If we consider the x axis, which intersects the cylinder at $\pm a$ and along which the undiffracted pulse extends from $+c\tau$ to $-c\tau$, a composite representation, formed from the one-term inner and outer expansions [cf. Eq. (5.34), Ref. 6], yields

$$P \sim \left[H\left(1 - \frac{x}{c\tau}\right) - H\left(-1 - \frac{x}{c\tau}\right)\right] \times \left[1 - \frac{\ln (|x|/c\tau)}{\ln R}\right]. \tag{57}$$

VI. ARBITRARY CAVITY SHAPE

We consider first the case of plane-wave scattering by a cavity of arbitrary shape and with a characteristic length l. The inner expansion is a solution of the Dirichlet problem for the region exterior to the cavity. In addition, the required solution must have logarithmic growth at large distances from the cavity in order that the leading terms of the inner and outer expansions match. We characterize the inner solution as

$$\psi \sim \Delta(\epsilon)[\ln (r/l) + F(r, \theta; l)]^{\epsilon=kl\to 0}_{l \text{ fixed}}, \tag{58}$$

where F is a function which is bounded in the exterior region and which cancels the fundamental solution $\ln r$ along the cavity boundary. The bracketed quantity in Eq. (58) is simply the Green's function and may be found for many exterior domains by conformal mapping.[7] An example of such a calculation will be given later in this section for the case of an ellipse.

The matching of the one-term inner and outer expansions follows precisely the development given by Eqs. (17) and (18), with the result

$$\Delta(\epsilon) = 1/\ln (\epsilon)^{-1}. \tag{59}$$

The two-term outer expansion is

$$\psi \sim e^{i\tilde{\rho}\cos\theta} + A_0(\epsilon)H_0^{(1)}(\tilde{\rho}), \tag{60}$$

where $A_0(\epsilon)$ is determined by matching with the inner expansion. As we have just indicated, the $O(1)$ term of the inner expansion is zero in the two-dimensional problem, the leading term being of $O(1/\ln \epsilon)$. Thus the source length $A_0(\epsilon)$ is found by matching to be

$$A_0(\epsilon) = i\frac{\pi}{2}\frac{1}{\ln \epsilon}. \tag{61}$$

The following remarks may now be made with regard to the inner and outer expansions to $O(1/\ln \epsilon)$. First, Eqs. (59) and (61) are independent of the cavity shape, which governs only the function F of the inner expansion. Second, the gauge function $\Delta(\epsilon)$ and the source strength $A_0(\epsilon)$ are determined, in rough measure, by the relative size of the cavity with respect to the wavelength. By rough measure we refer to the fact that the particular choice of characteristic length (e.g., radius or diameter for a circle, major or minor axis or semiaxis for an ellipse) is arbitrary as long as these respective lengths are of the same order. This is clear since any multiple of ϵ in Eq. (59) or (61) must be regarded as a change of $O(1/\ln^2 \epsilon)$. We therefore consider the next term of the inner expansion, which is of this order, and which must be influenced by the particular choice of characteristic length.

The next term of the inner expansion, κ,

$$\psi \sim \left[1\Big/\left(\ln\frac{1}{\epsilon} + \kappa\right)\right]\left[\ln\frac{r}{l} + F(r, \theta; l)\right], \tag{62}$$

is determined by rewriting Eq. (62) in outer variables, expanding for small ϵ to $O(1/\ln \epsilon)$ and matching with the inner expansion to $O(1/\ln^2 \epsilon)$ of the outer expansion to $O(1/\ln \epsilon)$, namely,

$$\frac{1}{\ln (\epsilon)^{-1}}\left[\ln\frac{r}{l} + \ln \tfrac{1}{2} + C - i\frac{\pi}{2}\right]. \tag{63}$$

It is apparent from Eq. (62) that any constant appearing in the function $F(r, \theta; l)$ will be retained after the indicated expansion and will influence the value of κ. Moreover, a change in the reference length l will change the value of the constant appearing in F so as to satisfy the boundary condition on the

[7] G. F. Carrier, M. Krook, and C. E. Pearson, *Functions of a Complex Variable: Theory and Technique* (McGraw-Hill Book Co., New York, 1966).

surface of the cylinder. In order to illustrate this point we consider the value of κ given by Eq. (23) for a circle of radius a, where the characteristic length was taken to be a and where F was identically zero. If the characteristic length had been taken as the diameter, $l = 2a$, then the function F would have assumed the value $F = \ln 2$ and the value of κ would have been larger by the same amount. The next term of the outer expansion, which is $O(1/\ln^2 \epsilon)$, also reflects the particular choice of characteristic cavity length because it is obtained by matching with the inner expansion to the same order. We may summarize our remarks by stating that to $O(1/\ln^2 \epsilon)$ the effect of cavity shape resides in the function $F(r, \theta; l)$ of the inner expansion only, while the effect of cavity size influences the coefficients of both expansions in a rough way to $O(1/\ln \epsilon)$ and in a precise way to $O(1/\ln^2 \epsilon)$.

In order to utilize the previous computed value for κ, Eq. (23), for any cavity shape we must seek a characteristic dimension l, associated with that shape, which will render the constant in the function $F(r, \theta; l)$ identically zero. This choice of characteristic dimension will also allow us to use the result, Eq. (25), for the outer region where the cavity has the effect of an equivalent circle of radius l. The determination of such a length may be accomplished by conformal mapping and will be illustrated for the case of a family of confocal ellipses with major and minor semiaxes

$$a_0 = l + l^{-1}, \quad b_0 = l - l^{-1}, \tag{64a}$$

respectively. The foci are on the x axis at the points $x = \pm 2$ and the equation of the boundary is

$$(x^2/a_0^2) + (y^2/b_0^2) = 1. \tag{64b}$$

A circle of radius l, considered to lie in the complex ζ plane, may be mapped onto the ellipse of Eq. (59), considered to be in the Z plane, by the transformation

$$Z = \zeta + \zeta^{-1}, \tag{65a}$$

which has as its inverse

$$\zeta = \frac{Z}{2}\left[1 \pm \left(1 - \left(\frac{2}{Z}\right)^2\right)^{\frac{1}{2}}\right]. \tag{65b}$$

We choose the branch corresponding to the positive square root, with a branch cut between $Z = \pm 2$, so that the point $\zeta \to \infty$ maps into the point $Z \to \infty$. We may regard the desired solution as the real part of a complex potential F, which in the ζ plane is given by

$$F(\zeta) = \ln (\zeta/l). \tag{66a}$$

The solution in the Z plane is, therefore,

$$\operatorname{Re} F(Z) = \ln \frac{r}{l} + \operatorname{Re} \ln \frac{1}{2}\left[1 + \left(1 - \left(\frac{2}{Z}\right)^2\right)^{\frac{1}{2}}\right], \tag{66b}$$

which has the desired behavior as $Z \to \infty$. It is convenient to introduce elliptic coordinates

$$x = 2 \cosh \xi \cos \eta,$$
$$y = 2 \sinh \xi \cos \eta, \tag{67}$$

which reduce Eq. (58) to

$$\psi \sim \Delta(\epsilon)[\xi + \ln (a)^{-1}]_{l \text{ fixed}}^{\xi \to 0}, \tag{68a}$$

where the equipotential curves are the ellipses

$$(x^2/\cosh^2 \xi) + (y^2/\sinh^2 \xi) = 4 \tag{68b}$$

and the cavity boundary is given by

$$\xi_0 = \ln l. \tag{68c}$$

The choice of l for the characteristic cavity dimension allows us to use the value for κ given by Eq. (23) and to characterize the ellipse at large distances as an equivalent circle of radius l.

For the case of pulse scattering by a cavity of arbitrary shape, the inner expansion has the form

$$P \sim \frac{P_{\text{inc}}(T_0)}{\ln (R)^{-1} + \kappa(T_0)}\left[\ln \frac{r}{l} + F(r, \theta; l)\right], \tag{69a}$$

where

$$R = l/c\tau \tag{69b}$$

and where $\kappa(T_0)$ may be determined by matching with the two-term outer expansion. The second term of the latter expansion is a Fourier synthesis which employs the plane-wave solution at long wavelengths, Eq. (48), and is independent of cavity shape. Therefore, if we employ the appropriate characteristic length l, discussed above, we may use the results already obtained for $\kappa(T_0)$ which depend only on the form of the incident pulse.

ACKNOWLEDGMENTS

This work was supported by the Lockheed Palo Alto Research Laboratory. The author wishes to thank three professors at Stanford University: Milton Van Dyke, who pointed out the singular nature of the problem and offered several useful suggestions, I-Dee Chang, for many helpful discussions, and Harold Levine for a great deal of help and encouragement.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Self-Consistent Approximations in Many-Body Systems

M. REVZEN* AND L. E. H. TRAINOR
University of Toronto, Toronto, Canada

(Received 14 September 1968)

A new stationary property of the grand canonical potential is presented. This property is used to define a class of self-consistent approximations which is particularly appropriate for the so-called ladder approximation. The conditions which guarantee self-consistency are only sufficient. A comparison is made with the already-known stationary properties related to Hartree–Fock and random-phase approximations. Remarks are made on the possibility of a collective excitation associated with the formalism.

I. INTRODUCTION

It is well known[1,2] that the grand canonical potential Ω is stationary with respect to variations of the proper self-energy Σ. This property has proved to be of particular importance in the study of many-body problems; e.g., it has been used effectively[3] in establishing a microscopic theory of Fermi liquids. In a more general context, it was used by Baym[4] to describe a certain class of self-consistent approximations (henceforth, SCA). Subsequently, Revzen[5] rephrased Baym's SCA in a more diagrammatic language and related it to the formulations of the exact many-body problem of Balian, Bloch, and DeDominicis; in particular, he showed that many results valid for the exact system, e.g., the Hugenholz–Van Hove theorem, are likewise valid in SCA. (Reference 5 forms part I of the present series of papers.) Using a second stationary property of Ω related to stability under fluctuations in the density–density correlation function,[6] Shlidor and Revzen[7] (Paper II of the present series) defined a second class of SCA which is particularly appropriate to a discussion of the random phase approximation (RPA).

In the present paper we introduce a third stationary property of Ω, this time related to stability with respect to variations in the dressed propagator describing the center-of-mass motion of two particles in the medium. This stationary property leads us to define a third class of SCA which is especially convenient for the discussion of the usual ladder approximation (LA).

The new stationary property is developed in Sec. II and applied in Sec. III to define a new class of self-consistent approximations. In Sec. IV we discuss all three classes of SCA from a unified point of view and speculate on the possible completeness of our description.

II. STATIONARY PROPERTY OF THE GRAND CANONICAL POTENTIAL

The grand canonical potential is defined by the expression

$$\Omega = -(\beta^{-1}) \log \{\mathrm{Tr}\,[e^{-\beta(H-\mu N)}]\} \tag{1}$$

with the same notation as in II. We write the Hamiltonian in the plane-wave representation in the form

$$H = \sum_k \epsilon_k a_k^+ a_k + \sum_{k,k',K} v(k, k') a_{k+K}^+ a_{-k}^+ a_{-k'} a_{k'+K}, \tag{2}$$

where K plays the role of the center-of-mass momentum of the colliding particles; spin indices, wherever appropriate, are omitted as a matter of convenience. Since $v(k, k')$ is a function only of the momentum transfer $q = k - k'$ for central interactions, we can expand it as a sum of separable potentials[8] $v_\sigma(k')$:

$$v(k, k') = \sum_\sigma v_\sigma^*(k) v_\sigma(k'). \tag{3}$$

Introducing potential-normalized momentum creation and annihilation operators

$$A_K^{\sigma+}(u) = \sum_k v_\sigma^*(k) a_{k+K}^+(u) a_{-k}^+(u) \tag{4a}$$

and

$$A_K^\sigma(u) = \sum_k v_\sigma(k) a_{-k}(u) a_{k+K}(u), \tag{4b}$$

the Hamiltonian can be rewritten in the form

$$H = \sum_k \epsilon_k a_k^+ a_k + \sum_K \sum_\sigma A_K^{\sigma+} A_K^\sigma. \tag{5}$$

* On leave from the Technion-Israel Institute of Technology, Haifa, Israel.

[1] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).

[2] C. Bloch, Physica **26**, 562 (1960).

[3] Proofs of the Landau theory of Fermi liquids are based on this variational property, e.g., in D. Pines and P. Nozières, *Theory of Quantum Liquids* (W. A. Benjamin, Inc., New York, 1966), Vol. I.

[4] G. Baym, Phys. Rev. **127**, 1391 (1962).

[5] M. Revzen, J. Math. Phys. **6**, 450 (1965). This paper is referred to as I.

[6] C. DeDominicis and P. Martin, J. Math. Phys. **5**, 14 (1964).

[7] O. Shlidor and M. Revzen, submitted to J. Math. Phys. This paper is referred to as II.

[8] D. J. Thouless, Ann. Phys. (N.Y.) **10**, 553 (1960). H. U. Everts, Z. Physik **199**, 211 (1966).

In these expressions, u is the thermal time variable restricted to the range $0 \leq u \leq \beta$ and the time-dependent operators are given by

$$a_k(u) = e^{u(H-\mu N)} a_k e^{-u(H-\mu N)}. \tag{6}$$

We now define a basic correlation function $C_K^{\sigma\sigma'}$, which, in a sense to be defined later, is related to the propagator for the center-of-mass momentum K:

$$C_K^{\sigma\sigma'}(u - u') = \langle T[A_K^{\sigma}(u) A_K^{\sigma'+}(u')] \rangle. \tag{7}$$

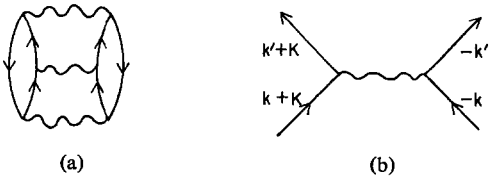
Here T is the thermal time-ordering operator and the expectation value is taken in the grand canonical ensemble (gce),

$$\langle C \rangle = \mathrm{Tr}\,(e^{-\beta(H-\mu N)} C)/\mathrm{Tr}\,(e^{-\beta(H-\mu N)}). \tag{8}$$

We note that for momentum-conserving potentials, $\langle A_K^{\sigma+} A_{K'}^{\sigma} \rangle = \delta_{KK'}$, so that the correlation function C is diagonal in the center-of-mass momentum K.

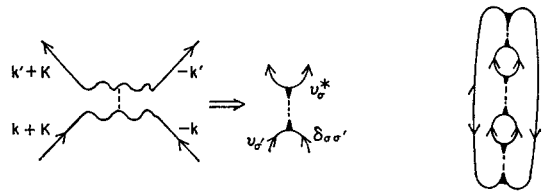
We are primarily concerned here with the diagrammatic expansion[1] of Ω. In order to develop the properties of the correlation function $C_K^{\sigma\sigma'}$ defined in Eq. (7), we introduce a new class of "skeleton diagrams" as follows: Each potential line in any diagram [wavy lines in Fig. 1(a)] has two particle lines entering it and two particle lines leaving it. By momentum conservation, the total momentum carried into a collision [K in Fig. 1(b)] equals the total momentum carried away. Now consider any diagram in the expansion for Ω. We shall call a diagram "skeleton" *if no two (or more) potential lines in the diagram have the same center-of-mass momentum associated with them by virtue of the conservation laws.* Diagrams which are not skeleton can be regarded as skeleton diagrams with insertions which conserve the center-of-mass momentum of a colliding pair.

In order to make this definition more transparent, we replace the usual diagrammatic representation by a new one in the following manner. Imagine each potential line (wavy line) in the usual representation sliced into two wavy lines joined by a dotted line, as in Fig. 2(a), in such a way that the incoming particle lines are attached to one wavy line and the outgoing particle lines are attached to the other. The former can then be associated with the annihilation operator



(a) (b)

FIG. 1. (a) A diagram that contributes to the grand canonical potential Ω. The wavy lines represent the matrix elements of the interaction and the directed lines represent free-particle propagators. (b) Momentum conservation ensures that the center-of-mass momentum K is the same before and after collision.



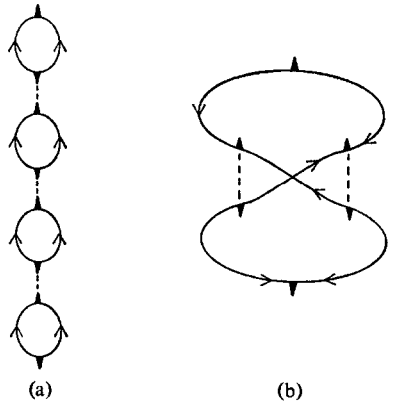
(a) (b)

FIG. 2. (a) Transformation of a two-particle collision diagram into the new language. The dotted lines represent $\delta_{\sigma\sigma'}$, the solid triangle $v_{\sigma'}$, and the inverted solid triangle v_σ^*. (b) The diagram of Fig. 1(a) transformed into the new language.

$A_K^{\sigma}(u)$ and the latter with the creation operator $A_K^{\sigma'+}(u)$, while the dotted line can be represented conveniently as the unit matrix $\delta_{\sigma\sigma'}$. It is now convenient to replace the dissected wavy lines by solid triangles (or arrowheads) in such a manner that the apex points into the dotted line while the base is connected to the particle lines; triangles with apex pointing downward accommodate incoming particle lines, triangles with apex pointing upward accommodate outgoing particle lines. With these conventions, the diagram in Fig. 1(a) is transformed into Fig. 2(b).

The concept of skeleton diagrams as we use it in this paper now becomes transparent from a geometrical point of view: a skeleton diagram is one which does not become disconnected when any two dotted lines are removed. The diagram in Fig. 2(b) is clearly not skeleton.

Our correlation function $C_K^{\sigma\sigma'}$ can also be represented by diagrams using this new terminology; diagrams corresponding to C are identical with those corresponding to Ω, except that two solid triangles are not joined to the rest of the diagram by dotted lines. (This situation is analogous to the usual case of diagrams for Green's functions where there are two free particle lines, and also to the case put forward in II where diagrams for the density–density correlation function have two heavy dots.) Two examples of diagrams for $C_K^{\sigma\sigma}$ are shown in Fig. 3; the diagram



(a) (b)

FIG. 3. Diagrams that contribute to $C_K^{\sigma\sigma'}(\xi_l)$: (a) a reducible (ladder) diagram; (b) an irreducible diagram.

in Fig. 3(a) is reducible,[9] while that in Fig. 3(b) is irreducible. If we label the sum of all irreducible contributions to $C_K^{\sigma\sigma'}$ by $S_K^{\sigma\sigma'}$, we can write

$$C_K^{\sigma\sigma'} = S_K^{\sigma\sigma'} + S_K^{\sigma\nu}\delta_{\nu\nu'}S_K^{\nu'\sigma'} + S_K^{\sigma\nu}\delta_{\nu\nu'}S_K^{\nu'\omega}\delta_{\omega\omega'}S^{\omega'\sigma'} + \cdots$$
$$= [S_K/(1 - S_K)]^{\sigma\sigma'} = S_K^{\sigma\nu}\delta_{\nu\nu'}I_K^{\nu'\sigma'}, \quad (9)$$

where the summation convention is used and where $I_K = 1/(1 - S_K)$ can be regarded as a sort of "propagator" which dresses up the δ function (dotted lines) and corresponds to the propagation of center-of-mass momentum.

From this point we follow closely the procedures used in Refs. 1 and 4. Extending the range of definition of various functions of the thermal variable by assuming a periodicity β, we can go over to an "energy" representation by expanding ${}^{(n)}C_K^{\sigma\sigma'}$ as a Fourier series, where ${}^{(n)}C_K^{\sigma\sigma'}$ is the sum of all diagrams of C having $2n + 2$ solid triangles, $2n$ of which are connected in pairs by dotted lines (corresponding to n internal interaction lines). We denote the corresponding Fourier coefficients by ${}^{(n)}C_K^{\sigma\sigma'}(\xi_l)$, where $\xi_l = 2l\pi i/\beta + \mu$, $l = 0, \pm 1, \cdots$, for bosons.

Clearly ${}^{(n)}C_K^{\sigma\sigma'}$, which we now represent by diagrams such as those in Fig. 3, can be obtained by removing in turn one of the various dotted lines in the $(n + 1)$th-order diagrams for Ω. It follows[1,7] that the contribution to the thermodynamic potential of order $(n + 1)$ in the interaction is given by

$$(\Omega - \Omega_0)_{(n+1)} = -\frac{1}{2\beta(n+1)}\sum_K\sum_l \delta_{\sigma\sigma'}^{(n)}C_K^{\sigma\sigma'}(\xi_l). \quad (10)$$

The $(n + 1)$-dependence can be removed formally in the usual fashion by integrating over a parameter λ which characterizes the strength of the interaction [i.e., by replacing $v_\sigma(k)$ everywhere by $(\lambda)^{\frac{1}{2}}v_\sigma(k)$]. In this way we obtain

$$\Omega(\lambda) = \Omega_0 - \frac{1}{2\beta}\sum_K\sum_l\sum_{\sigma,\nu}\int_0^\lambda \frac{d\lambda'}{\lambda'}\delta_{\nu\nu'}S_K^{\sigma\nu}(\xi_l)I_K^{\nu'\sigma}(\xi_l). \quad (11)$$

From Eq. (11), and also directly from its definition,

$$I_K^{\sigma\sigma'} = \delta^{\sigma\sigma'} + \sum_{\nu'}\delta_{\sigma\nu}S_K^{\nu\nu'}I_K^{\nu'\sigma'}, \quad (12)$$

one can interpret $I_K^{\sigma\sigma'}$ as a "dressed up" dotted interaction line. This observation enables us to obtain Ω as an explicit functional of $S_K^{\sigma\sigma}$ in much the same way as $\Omega(G_k(\xi_l))$ in Ref. 1 and $\Omega(W_k(\xi_l))$ in Ref. 7. We first define $R'(\lambda)$ as the sum of all skeleton (in the present sense) diagrams contributing to $\Omega - \Omega_0$ in which each dotted line $\delta_{\sigma\sigma'}$ has been replaced by $I_K^{\sigma\sigma'}$. It follows that

$$R'(\lambda) = -\frac{1}{2\beta}\sum_n\sum_K\sum_l\sum_\sigma\frac{1}{(n+1)}[{}^{(n)}S_K(\xi_l)I_K(\xi_l)]^{\sigma\sigma}, \quad (13)$$

where ${}^{(n)}S_K^{\sigma\sigma}$ is the sum of nth-order skeleton diagrams corresponding to ${}^{(n)}C_K^{\sigma\sigma}$. This definition of $R'(\lambda)$ implies that

$$\frac{\partial R'}{\partial S_K^{\sigma\sigma'}(\xi_l)} = -\left(S\frac{\partial}{\partial S}\frac{1}{1-S}\right)_K^{\sigma\sigma'}$$
$$= -[C_K(\xi_l)I_K(\xi_l)]^{\sigma\sigma'}. \quad (14)$$

Furthermore, from the definition

$$R''(\lambda) = \frac{1}{2\beta}\sum_K\sum_l\sum_\sigma(\{\ln[-1 + S_K(\xi_l)]\}^{\sigma\sigma} + \{S_K(\xi_l)I_k(\xi_l)\}^{\sigma\sigma}), \quad (15)$$

we have

$$\frac{\partial R''}{\partial S_K(\xi_l)^{\sigma\sigma'}} = +[C_K(\xi_l)I_K(\xi_l)]^{\sigma\sigma'}. \quad (16)$$

Hence, we have the stationary property

$$\frac{\partial R}{\partial S_K(\xi_l)^{\sigma\sigma'}} = 0, \quad (17)$$

where $R = R' + R''$.

Now it is easy to show that $R = \Omega - \Omega_0$. If we calculate the derivative $\partial R/\partial\lambda$, only the explicit dependence is involved, since the implicit dependence of R on λ through S_K (or equivalently I_K) gives no contribution by virtue of Eq. (17). Since an nth-order contribution from ${}^{(n)}S_K$ in Eq. (13) contributes $(n + 1)$ powers of λ, the $(n + 1)$-dependence vanishes in $\partial R/\partial\lambda$ and the summation over n then leads to

$$\lambda\frac{\partial R}{\partial\lambda} = -\frac{1}{2\beta}\sum_K\sum_l\sum_\sigma\int_0^\lambda\frac{d\lambda'}{\lambda'}\delta_{\nu\nu'}S_K^{\sigma\nu}(\xi_l)I_k^{\nu'\sigma}(\xi_l)$$
$$= \lambda\frac{\partial(\Omega - \Omega_0)}{\partial\lambda}. \quad (18)$$

From $R(\lambda = 0) = 0$, it follows that

$$R = \Omega - \Omega_0 \quad (19)$$

and, hence, that

$$\frac{\partial\Omega}{\partial S_K^{\sigma\sigma'}(\xi_l)} = 0. \quad (20)$$

This is the new stationary property for Ω which we shall use in the next section to define a new class of SCA particularly appropriate to the ladder approximation.

III. SELF-CONSISTENT APPROXIMATIONS OF THE THIRD CLASS

We shall refer to SCA based on the stationary property of Ω with respect to the Green functions as

[9] By "reducible" we mean a natural extension of the idea of skeleton diagram as used in this work.

belonging to class I and to SCA based on the stationary property with respect to the density–density correlation function as belonging to class II. The class developed in the present context will be referred to as III.

Consider now any subset of the totality of skeleton diagrams of Ω (skeleton in the sense defined in Sec. II). By definition these diagrams remain connected when any pair of dotted lines is removed. Let S_A be the sum of all diagrams obtained by breaking pairs of dotted lines in the subset in all possible ways and replacing all unbroken dotted lines $\delta_{\sigma\sigma'}$ by $I_A^{\sigma\sigma'}$ (index K understood), where $I_A^{\sigma\sigma'}$ is defined by the relations

$$C_A^{\sigma\sigma'} = [S_A(1 - S_A)^{-1}]^{\sigma\sigma'} \tag{21}$$

and

$$I_A^{\sigma\sigma'} = [1/(1 - S_A)]^{\sigma\sigma'}. \tag{22}$$

Since all functional relationships are preserved in this approximation, we obtain, in one-to-one correspondence with the arguments in Sec. II,

$$\frac{\partial \Omega_A}{\partial S_A^{\sigma\sigma'}(\xi_l)} = 0, \tag{23}$$

where Ω_A is the grand canonical potential corresponding to the subset of diagrams obtained by closing all $C_A^{\sigma\sigma'}$ diagrams, viz., to nth-order

$$(\Omega_A - \Omega_0)_{(n+1)} = -\frac{1}{2\beta(n+1)} \sum_K \sum_l \delta_{\sigma\sigma'}{}^{(n)} C_{AK}^{\sigma\sigma'}(\xi_l). \tag{24}$$

Equation (23) guarantees self-consistency, viz., that all relationships derived from the functional forms of Ω are preserved in the SCA based on Eq. (24). We illustrate this by calculating the particle number in our gce [cf. Eq. (24) of II]:

$$\langle N \rangle = -\frac{\partial \Omega}{\partial \mu} = -\frac{\partial R}{\partial \mu} - \frac{\partial \Omega_0}{\partial \mu}. \tag{25}$$

Now, the stationary property (23), just as (20), guarantees that $\partial R_A''/\partial\mu$ will cancel out that part of $\partial R_A'/\partial\mu$ which arises purely through the dependence of R_A' on μ by virtue of the dependence of S_A on μ. Hence, one need consider only the dependence of R' on μ through the free propagators, viz.,

$$\frac{\partial R_A}{\partial \mu} = \sum_{n=0} \sum_{k,l} \frac{\partial R_A'^{(n+1)}}{\partial G_{Ak}^0(\xi_l)} \frac{\partial G_{AK}^0(\xi_l)}{\partial \mu}, \tag{26}$$

where $R'^{(n+1)}$ signified the $(n+1)$th-order contribution to R'. From (25) and (27) one obtains [see Eq. (25) of II]

$$\langle N \rangle = \frac{1}{\beta} \sum_{k,l} G_{AK}(\xi_l). \tag{27}$$

In words, our approximation preserves the same sum rule for the particle number in terms of the approximate Green function as is obtained in the exact case using the exact Green function. This result illustrates again the advantages of an SCA based on preserving the functional relationships between Ω and the component functionals C, S, and I. Note that here (as in II) Σ is a functional of G_0 and not of G (as in I).

Just as the class II of SCA defined in II was natural for expressing the random phase approximation, so is the class III SCA defined in the present work natural for expressing the ladder approximation. By "natural," we mean that the RPA is most simply described as a class II SCA while the LA is most simply described as a class III SCA. (Likewise, class I SCA is a natural for the Hartree–Fock approximation.) In fact, the LA approximation regarded as SCA III consists of a single diagram for the (irreducible) set $S_K^{\sigma\sigma}(\xi_l)$ as shown in Fig. 4. The corresponding Ω_A then consists entirely of ladder diagrams. If one considers the LA using the Green's function method, not only does an infinite set of diagrams occur, but Ω_A corresponding to it must also contain Green's-function insertions, as illustrated in Fig. 5. These remarks are analogous to the corresponding ones which were made for the RPA in II.

FIG. 4. The diagram for $S_K^{\sigma\sigma'}(\xi_l)$ which gives, along with its topologically equivalent diagram, the basis for the SCA of type III which is equivalent to the usual ladder approximation.

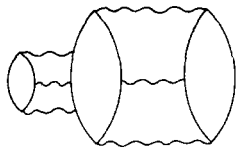


FIG. 5. In the Green's function formulation of the ladder approximation, diagrams of this type must be included along with that in Fig. 1(a).

IV. REMARKS AND CONCLUSIONS

In this paper we have obtained two results; the first is a new stationary property of the grand canonical potential Ω, the second is a new class of self-consistent approximations based on it which we refer to as class III. We conjecture at this point that classes I, II, and III exhaust the possible basic SCA, at least for normal systems. As a partial basis for this conjecture, we note that, for Hamiltonians corresponding to two-body forces, DeDominicis and Martin[6] (DDM) showed that Ω is stationary in gce with respect to variations in the time-independent two-body correlation function. The SCA developed in II and that developed here can be regarded as generalizations of the work of DDM to time-dependent cases;

there seem to be no other simple and reasonable generalizations. Moreover, Kraichnan[10] has shown how to generate the Hartree–Fock, random phase and ladder approximations by using a stochastic model Hamiltonian. Clearly, within the framework of the stochastic model Hamiltonian theory used by Kraichnan, it should be a straightforward matter to prove the various stationary properties for the SCA that we used in I, II, and in the present paper. Now Kraichnan remarks that no other approximations can be treated in a simple manner using his approach. In this sense, his approach also singles out the same three SCA as discussed here.

Finally, we draw attention to the basic similarity of the treatments leading to SCA of types I, II, and III. Analogous to the Green function G and the irreducible self-energy Σ of type I, we have the quantities U and W in type II, and I and S in the present type III. The following equations bear out this similarity; they are illustrated diagrammatically in Fig. 6 (where I is represented by a line with crosses):

$$G = G_0 + G_0 \cdot \Sigma \cdot G, \tag{28a}$$

$$U = v + v \cdot W \cdot U, \tag{28b}$$

$$I = \delta + \delta \cdot S \cdot I. \tag{28c}$$

In the third of these equations, δ represents the unit matrix.

[10] R. H. Kraichnan, J. Math. Phys. 3, 475 (1962).

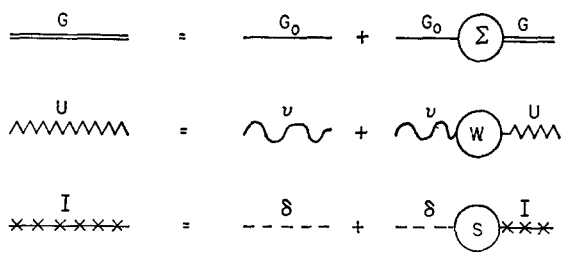


FIG. 6. Dyson's equation for the dressed Green's function is compared schematically with its analogs, viz., the momentum-transfer propagator U and the center-of-mass propagator I.

The poles for the quantities G and U in Eqs. (28a) and (28b) are, respectively, the single-particle excitation branch and the density oscillation (collective) branch of the excitation spectrum of the system. (The latter branch corresponds to phonons when the potential is short-ranged, and to plasmons for the Coulomb potential.) In an analogous manner, one would expect the poles of I [Eq. (28c)] to correspond to some kind of collective excitation. For fermions, this is related to the Cooper instability for certain potentials in the low-K limit. More generally, we expect it to be related to zero sound. We can make no remarks at this time for the case of a system of bosons.

ACKNOWLEDGMENT

One of us (M. R.) wishes to acknowledge several helpful remarks of O. Shlidor.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 10, NUMBER 9 SEPTEMBER 1969

Wiener–Hopf Method and Generalized Integral Transforms

A. BASSETTO AND F. PACCANONI
Istituto di Fisica dell'Università di Padova, Istituto Nazionale di Fisica Nucleare—Sezione di Padova, Padua, Italy

(Received 25 December 1967)

We consider the class of singular integral equations that can be solved by means of the Wiener–Hopf technique. The resolvent is given as a dispersion relation in the plane of the parameter λ and some physical applications are discussed.

1. INTRODUCTION

In the last years several problems have been considered in the framework of the elementary-particle physics that require the solution of singular integral equations. We recall as typical examples the "new strip approximation"[1] and the scattering processes where higher-spin particles are exchanged[2–4] or, in general, where singular potentials are involved.[5] All these examples are characterized by equations that can be brought to the Fredholm form once the singular part has been solved by means of the Wiener–Hopf technique.

The solution one obtains is a multivalued function in the cut coupling constant plane; among the various determinations it is possible to choose the one derived from a resolvent which is regular and approaches the kernel in the weak coupling limit. In this way one gets for the amplitude a unique expression that allows a perturbative expansion for small coupling and is suggested on the basis of unitarity conditions.[3,6] However, the resolvent is rather cumbersome from an analytical point of view as well as from a computational one; moreover, it does not generally allow a clear insight into the coupling constant plane singularities.

In particular cases[3,5] the existence of an integral transform that diagonalizes the equation greatly simplifies the structure of the result. The resolvent is given as an integral over the continuous spectrum of the kernel in close analogy with the Hilbert–Schmidt case, where it is expressed as a series over the discrete spectrum of eigenvalues. This procedure, however, is confined to the class of the usual integral transforms, and no general prescription exists for choosing among them. The aim of our paper is to derive for a special class of Wiener–Hopf soluble problems an expression for the resolvent that exhibits the spectrum of the kernel even for the equations that cannot be diagonalized by means of known transforms. As we see below, the discontinuity of the resolvent on the cut is related to the solutions of the homogeneous problem. Furthermore, in this new form, the resolvent can be readily continued in the cut coupling constant plane.

The interest of our procedure is obviously not confined to the field of elementary particles; indeed it can apply to several problems in other branches of physics.[7]

2. THE METHOD

In the sequel we follow the notations used in Ref. 8. As is well known, the Wiener–Hopf method applies to equations with a kernel depending on a difference when the interval of integration is $(0, +\infty)$:

$$\phi(x) = f(x) + \lambda \int_0^\infty K(x - t)\phi(t)\, dt. \qquad (1)$$

We seek a $\phi(x)$ that satisfies Eq. (1) for all real x, with $f(x) = 0$ for $x < 0$ and continuous for $x \geq 0$. We assume that $K(x)$ is continuous and that, for some real r, the functions $K(x)e^{-rx}$, $f(x)^{-rx}$, and $\phi(x)e^{-rx}$ are absolutely integrable for $-\infty < x < +\infty$, the first two having in addition a finite number of intervals of increase and decrease.[8] Let us call $L(s)$ the two-sided Laplace transform of the kernel $K(x)$.

We are led to a nonhomogeneous Hilbert problem for a contour belonging to the strip of regularity of $L(s)$ $(a < \mathrm{Re}\, s < b)$:

$$\Phi^+(s) = [1 - \lambda L(s)]\Phi^-(s) + F(s), \qquad (2)$$

Φ^+, $-\Phi^-$ being the Laplace transforms of $\phi(x)$ when

[1] G. F. Chew, Phys. Rev. **130**, 1264 (1963); D. C. Teplitz and V. L. Teplitz, Phys. Rev. **137**, B136, B142 (1965).
[2] K. Dietz and G. Domokos, Phys. Letters **11**, 91 (1964); G. Auberson and G. Wanders, Phys. Letters **15**, 61 (1965); D. Morgan, Nuovo Cimento **36**, 813 (1965); A. P. Contogouris, Nuovo Cimento **44**, 927 (1966).
[3] D. Atkinson and A. P. Contogouris, Nuovo Cimento **39**, 1082, 1102 (1965); A. Bassetto and F. Paccanoni, Nuovo Cimento **44**, 1139 (1966); D. Atkinson, J. Math. Phys. **7**, 1607 (1966).
[4] A. Bassetto, P. Campogalliani, and F. Paccanoni, Nuovo Cimento **54**, 897 (1968).
[5] S. Ciulli, Gr. Ghika, M. Stihi, and M. Visinescu, Phys. Rev. **154**, 1345 (1967).
[6] A. P. Contogouris and A. Martin, Nuovo Cimento **49**, A61 (1967).
[7] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953).
[8] V. I. Smirnov, *Higher Mathematics* (Pergamon Press, Ltd., London, 1964).

$x < 0$ and $x > 0$, respectively, and F the transform of the known term $f(x)$. The standard way of solving Eq. (2) is to consider first the corresponding homogeneous problem

$$\Phi_0^+(s) = [1 - \lambda L(s)]\Phi_0^-(s) \qquad (3)$$

and, once Φ_0^+ and Φ_0^- are known, to use the Cauchy theorem for evaluating $\Phi(s)$.

In order to get a simple analytical structure of the solution in the variable λ, we confine ourselves to the case when only two zeros of $1 - \lambda L(s)$, $s_1(\lambda)$, and $s_2(\lambda)$, enter the strip. $a \leq \mathrm{Re}\, s \leq b$, where $a = s_1(0)$ and $b = s_2(0)$, and move, as λ grows from 0 to $+\infty$, as shown in Fig. 1. In the weak coupling limit, two solutions Φ_0^+ and Φ_0^- can be obtained, free from zeros

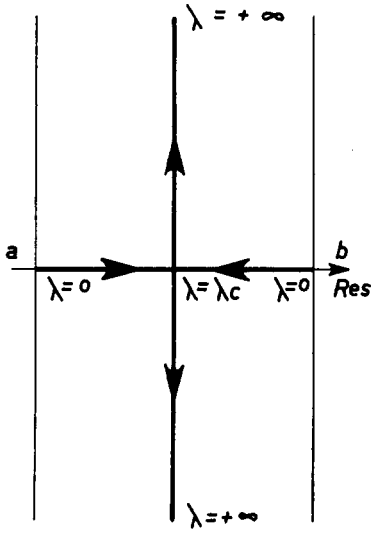


FIG. 1. Paths of the zeros of $1 - \lambda L(s)$ in the strip $a < \mathrm{Re}\, s < b$ as λ grows from 0 to $+\infty$.

and poles in the half-planes $\mathrm{Re}\, s \leq \mathrm{Re}\, s_2$ and $\mathrm{Re}\, s \geq \mathrm{Re}\, s_1$, respectively, and with the following asymptotic behavior in their domain of regularity:

$$\lim_{|s|\to\infty} \Phi_0^{\pm} = 1.$$

Thus, when $\mathrm{Re}\, s_1 < \mathrm{Re}\, s_2$, there is a common strip of regularity where we choose the contour C for solving Eqs. (2) and (3). As λ grows, this strip shrinks and eventually the two zeros pinch the contour C:

$$s_1(\lambda_c) = s_2(\lambda_c) = s_p.$$

One can easily recognize that the resolvent of Eq. (1), defined by the expression

$$\phi(x) = f(x) + \lambda \int_0^{\infty} R(x, y, \lambda) f(y)\, dy, \qquad (4)$$

has a branch point when $\lambda = \lambda_c$. In fact, when $\lambda > \lambda_c$ we can choose Φ_0^+ and Φ_0^- in two different ways, giving to λ a positive or negative small imaginary part. This procedure gives rise to different branches of the resolvent and is completely equivalent to keep

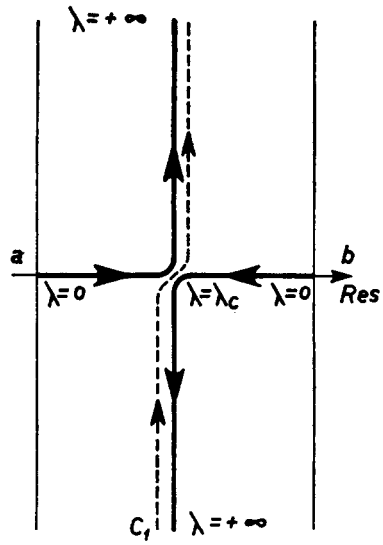


FIG. 2. Deformed contour of integration C_1 corresponding to the first branch of the resolvent for $\lambda > \lambda_c$.

λ real and to deform suitably the contour C as shown in Figs. 2 and 3. Both these determinations are obtained as analytical continuations from the weak coupling region where the resolvent is regular. We notice, furthermore, that it is also unique because there is no variation in the phase of $\log [1 - \lambda L(s)]$ along the contour C which we have considered.[8]

We have thus shown that the resolvent is cut in the λ plane from λ_c to infinity and it is now an easy matter to evaluate its discontinuity. To this end we recall the expression for the resolvent[8]:

$$R_i(x, y; \lambda) = \frac{1}{4\pi^2} \int_T e^{sx} \Phi_{0i}^-(s)\, ds \int_{C_i} \frac{e^{-ry} L(\tau)}{(\tau - s)\Phi_{0i}^+(\tau)}\, d\tau, \qquad i = 1, 2, \quad (5)$$

where T is the contour of the inverse Laplace transform to the right of C_i and the term i refers to the different continuations in Figs. 2 and 3, respectively.

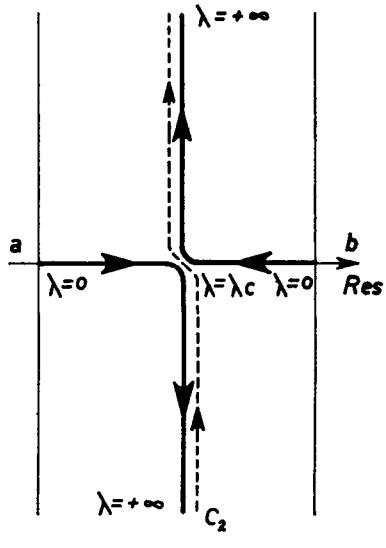


FIG. 3. Deformed contour of integration C_2 corresponding to the second branch of the resolvent for $\lambda > \lambda_c$.

It is obvious that R_1 and R_2 coincide for $\lambda < \lambda_c$. In the situation represented in Fig. 2, the zero s_1 acquires a positive imaginary part $s_1 = s_p + i\gamma(\lambda)$; whereas in the other case (Fig. 3), $s_1 = s_p - i\gamma(\lambda)$. The zero s_2 for $\lambda > \lambda_c$ satisfies the relationship $s_2 = s_{1*}$.

The $\Phi_{02}^{\pm}$ are related to the functions $\Phi_{01}^{\pm}$ by means of the following equations:

$$\Phi_{02}^{\pm} = \Phi_{01}^{\pm} \cdot g(s), \tag{6}$$

with

$$g(s) = (s - s_p - i\gamma)/(s - s_p + i\gamma).$$

From Eqs. (5) and (6) we get

$$R_2 = \frac{1}{4\pi^2} \int_T e^{sx} \Phi_{01}^{-}(s)\, ds \int_{C_2} \frac{e^{-\tau y} L(\tau)}{\Phi_{01}^{+}(\tau)} \frac{d\tau}{\tau - s} \frac{g(s)}{g(\tau)}. \tag{7}$$

Since

$$g(s)/[g(\tau) \cdot (\tau - s)] = -2i\gamma/[(s - s_p + i\gamma)(\tau - s_p - i\gamma)] + 1/(\tau - s), \tag{8}$$

the discontinuity is

$$\begin{aligned} R_1 - R_2 &= \frac{2i\gamma}{4\pi^2} \int_T \frac{e^{sx}\Phi_{01}^{-}(s)}{s - s_p + i\gamma}\, ds \\ &\quad \times \int_{C_2} \frac{e^{-\tau y} L(\tau)}{\tau - s_p - i\gamma} \frac{d\tau}{\Phi_{01}^{+}(\tau)} + \frac{1}{4\pi^2} \\ &\quad \times \int_T e^{sx}\Phi_{01}^{-}(s)\, ds \int_{C_1 - C_2} \frac{e^{-\tau y} L(\tau)\, d\tau}{\Phi_{01}^{+}(\tau)(\tau - s)} \\ &= \frac{2i\gamma(\lambda)}{\lambda} A(x, \lambda) B(y, \lambda), \end{aligned} \tag{9}$$

where

$$\begin{aligned} A(x, \lambda) &= \frac{1}{2\pi i} \int_T \frac{e^{sx}\Phi_{01}^{-}(s)}{s - s_p + i\gamma}\, ds, \\ B(y, \lambda) &= \frac{-1}{2\pi i} \int_D \frac{e^{-\tau y}\, d\tau}{\Phi_{01}^{+}(\tau)} \frac{1}{(\tau - s_p - i\gamma)}. \end{aligned} \tag{10}$$

The contour D is the straight line $\delta - i\infty \div \delta + i\infty$, with $a < \delta < s_p$. From the condition we imposed on the zeros of $1 - \lambda L(s)$ in the strip and the hypotheses we made in order to solve Eq. (1), it follows that the only quantity depending on λ in Eq. (5), that is, the ratio $\phi_{0i}^{-}(s, \lambda)/\phi_{0i}^{+}(\tau, \lambda)$, is finite in the limit $\lambda \to \lambda_c$ and vanishes uniformly when $|\lambda|$ goes to infinity.[9]

Owing to the uniform convergence of the integrals in Eq. (5), no contribution comes from the paths encircling the points $\lambda = \lambda_c$ and infinity if we write the resolvent as a dispersion relation in the variable λ.

Our final expression for the resolvent is

$$R(x, y; \lambda) = \frac{1}{\pi} \int_{\lambda_c}^{+\infty} \frac{\gamma(\lambda')}{\lambda'} \frac{A(x, \lambda')B(y, \lambda')}{\lambda' - \lambda}\, d\lambda'. \tag{11}$$

[9] E. C. Titchmarsh, *Theory of Fourier Integrals* (Oxford University Press, London, 1950).

Equation (11) exhibits in a clear way the analytical structure in the variable λ and looks much simpler when compared to Eq. (5), also from a computational point of view.

We would like to emphasize that the particular conditions we required in order to arrive at Eq. (11) are fulfilled in the most part of the practical problems that can be solved by the Wiener–Hopf technique. The extension of our procedure to more general kernels obviously requires a careful analysis of the zeros of the expression $1 - \lambda L(s)$ as well as of the asymptotic behavior of the resolvent in the λ plane. We notice, in addition, that the dispersion relation (11) allows a finite number of subtraction; in particular, if the resolvent is regular in weak coupling, it is easy to evaluate the "subtraction constants" that are the iterated kernels.

3. EXAMPLES

1. Let us consider first the kernel[7–9]

$$K(x - y) = e^{-|x-y|}, \tag{12}$$

whose two-sided Laplace transform is

$$L(s) = 2/(1 - s^2), \quad -1 < \mathrm{Re}\, s < 1. \tag{13}$$

The two zeros entering the strip are

$$s_{1,2} = \mp(1 - 2\lambda)^{\frac{1}{2}}, \tag{14}$$

and the pinch obviously occurs at $s_p = 0$ with $\lambda_c = \frac{1}{2}$. We obtain by inspection the solutions of the homogeneous Hilbert problem when $\lambda > \lambda_c$:

$$\Phi_{01}^{+} = (s + i\gamma)/(s - 1),$$
$$\Phi_{01}^{-} = (s + 1)/(s - i\gamma),$$

with

$$\gamma(\lambda) = (2\lambda - 1)^{\frac{1}{2}}, \tag{15}$$

and from Eq. (10) we get, finally,

$$A(z, \lambda) = B(z, \lambda) = \cos \gamma z + \sin(\gamma z)/\gamma. \tag{16}$$

2. The second example we consider is the singular kernel related to the continuation in the angular-momentum variable l ($0 < l \leq 1$) of the $I = 1$ pion–pion amplitude when a vector meson is exchanged[4]:

$$K(x - y) = -1/(2 \sin \pi l) \cdot (1 - e^{(l-1)(x-y)})/(1 - e^{(x-y)}) \tag{17}$$

in the interval $(0, +\infty)$.

The two-sided Laplace transform of $K(x)$ is

$$L(s) = \pi/[2 \sin \pi s \sin \pi(l - s)], \quad -1 < \mathrm{Re}\, s < l - 1. \tag{18}$$

It is easy to show that this kernel satisfies our requirements; in particular, the two zeros of $1 - \lambda L(s)$

entering the strip are

$$s_1 = -(3 - l)/2 - (i/2\pi)\log\{-\pi\lambda - \cos\pi l + i[1 - (\cos\pi l + \pi\lambda)^2]^{\frac{1}{2}}\},$$
$$s_2 = -(1 - l)/2 + (i/2\pi)\log\{-\pi\lambda - \cos\pi l + i[1 - (\cos\pi l + \pi\lambda)^2]^{\frac{1}{2}}\}, \quad (19)$$

and the pinch occurs at $s_p = l/2 - 1$, with $\lambda_c = (1 - \cos\pi l)/\pi$. The expression

$$\exp\left\{\frac{1}{2\pi i}\int_{C_1}\log[1 - \lambda L(z)]\frac{dz}{z - s}\right\} \quad (20)$$

gives the solutions to the homogeneous Hilbert problem $\Phi_{01}^{+}(s)$ and $\Phi_{01}^{-}(s)$ when s lies to the left and to the right of the contour C_1, respectively. By introducing Φ_{01}^{+}, Φ_{01}^{-}, and $\gamma(\lambda)$ as obtained from Eq. (19) in Eq. (10), one gets the resolvent in the form of Eq. (11).

The connection with the method of integral transform can be seen in the two particular cases $l = 1$ and $l = \frac{1}{2}$, where the functions $\Phi_{01}^{\pm}$ can be obtained explicitly.

(a) $l = 1$.

For $\lambda > \lambda_c = 2/\pi$:

$$\Phi_{01}^{+} = \Gamma^2(-s)/[\Gamma(\tfrac{1}{2} - s + i\gamma)\Gamma(-\tfrac{1}{2} - s - i\gamma)],$$
$$\Phi_{01}^{-} = \Gamma(s + \tfrac{3}{2} + i\gamma)\Gamma(s + \tfrac{1}{2} - i\gamma)/\Gamma^2(s + 1), \quad (21)$$
$$\gamma(\lambda) = \frac{1}{2\pi}\log\{\pi\lambda - 1 + [(\pi\lambda - 1)^2 - 1]^{\frac{1}{2}}\}.$$

It is now easy to perform the integration (10):

$$A(x, \lambda) = P_{-\frac{1}{2}-i\gamma}(2e^x - 1),$$
$$B(y, \lambda) = e^y P_{-\frac{1}{2}-i\gamma}(2e^y - 1). \quad (22)$$

The resolvent of Eq. (11) with A, B, and γ given in Eqs. (21) and (22) coincides with the one obtained by means of a shifted Mehler transform in Ref. 3. This equation also applies to a different physical context, that is, the "new strip approximation." [1,3]

(b) $l = \frac{1}{2}$.

For $\lambda > \lambda_c = 1/\pi$:

$$\Phi_{01}^{+} = \frac{\Gamma(-s)\Gamma(-\frac{1}{2} - s)}{\Gamma(-\frac{3}{4} - s - i\gamma)\Gamma(\frac{1}{4} - s + i\gamma)},$$
$$\Phi_{01}^{-} = \frac{\Gamma(s + \frac{7}{4} + i\gamma)\Gamma(s + \frac{3}{4} - i\gamma)}{\Gamma(s + \frac{3}{2})\Gamma(s + 1)}, \quad (23)$$
$$\gamma(\lambda) = \frac{1}{2\pi}\log[\pi\lambda + (\pi^2\lambda^2 - 1)^{\frac{1}{2}}].$$

The integrations (10) lead to

$$A(x, \lambda) = e^{-x/2}P_{-\frac{1}{2}-2i\gamma}(e^{x/2}),$$
$$B(y, \lambda) = e^y P_{-\frac{1}{2}-2i\gamma}(e^{y/2}). \quad (24)$$

Equations (11), (23), and (24) completely solve this case, which has several other physical applications, such as, for instance, singular potential scattering.[5] We notice finally that this equation is equivalent to the one of Dixon.[9]