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Certain Bootstraps and Related Equations

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Methods of deriving existence and nonexistence theorems for certain classes of nonlinear integral and other equations are discussed. The methods are illustrated by examples from high-energy physics of equations of the bootstrap type.

THE purpose of this note is to present methods of dealing with certain nonlinear integral and other equations which have been applied to a number of problems of physical interest[1,2] which arise in high-energy physics in connection with the bootstrap program.[3] The methods concern those equations which can be regarded as relations on a ring, or which are closely related to such equations. In the main text of this paper, we simply sketch the methods and discuss some new examples of physical interest. Since it is our purpose to write something intelligible to physicists as well as interesting to mathematicians, we relegate details to two series of extensive notes: one, indexed A1, A2 (Appendix A), explaining our terminology and containing also various points of physical interest; and the other, indexed B1, B2 (Appendix B), containing certain mathematical refinements.

Suppose first of all we are given a system of equations,

$$a + b + c \cdots = 0, \quad d + e + f \cdots = 0, \cdots, \tag{1}$$

where we have not bothered to distinguish between known and unknown quantities (A2), on a given commutative ring (A1).

The first possible method is the classical method of algebraic elimination theory (Ref. 4, Chap. XI) (A3).

Unfortunately, the conditions for applying this type of argument are too restrictive to apply to realistic physical problems, and if there is the slightest additional complication, the method does not work at all.

A method related to this, which we found useful, and of which we give an example below, is the following: let χ be a character (A4) of the given ring. Then the system (1) gives us

$$\chi(a) + \chi(b) + \chi(c) \cdots = 0, \qquad \chi(d) + \chi(e) + \chi(f) \cdots = 0, \cdots . \tag{2}$$

The system (2) is just a series of polynomial equations in ordinary numbers and can be solved easily. Then if there are sufficiently many (A5) characters, one can, in principle, reconstruct the solutions (B1). In particular, if the given ring is a topological algebra, one can use functional repre-

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[1] M. M. Broido, J. Math. Phys. **6**, 1702 (1965).

[2] M. M. Broido and J. G. Taylor, Phys. Rev. **147**, 993 (1966).

[3] G. F. Chew and S. C. Frautschi, Phys. Rev. Letters **7**, 349 (1961). A large bibliography appears in Ref. 2 above.

[4] B. L. van der Waerden, *Modern Algebra* (Frederick Ungar Publishing Company, New York, 1950).

sentation theory (A6). By arguments of this kind, one may not be able to get solutions, but, as we see below, existence and nonexistence proofs sometimes come out rather easily.

A second series of methods is that connected with fixed-point theorems of nonlinear analysis.[5] These have been further developed[6] and applied by Taylor[7] to problems similar to those discussed in this paper, and so we refer the reader to those references for discussion of such methods. They apply naturally to a rather different class of problems than the one we consider here and yield, in general, only an existence or nonexistence theorem.

Now suppose we are given the Eq. (1), but are *not* told on which ring they act (B2). The problem of constructing a space on which a given operator is a continuous mapping with certain properties is an old one in nonlinear functional analysis, apparently first considered by Schauder[8] but "has received little attention so far."[5] If there are *some* known functions in the equations, or if we have some sort of boundary conditions, such notions may be of help. Otherwise, we are completely at sea; "otherwise" covers many situations of genuinely physical interest. Under this heading come two methods which we discuss with examples and whose description and justification are the essential purpose of the present paper.

In the first of these methods, we make a definite set of assumptions about the underlying ring (B3). In practice, this is the analogy of selecting for a given (say) differential equation a definite class of boundary conditions (correctness class). We try to make the assumptions as general as possible, but it should be emphasized that any results obtained refer only to the particular class of rings chosen: such restrictions are an essential part of this methodology, particularly if one seeks a nonexistence theorem or a uniqueness theorem.

For instance, we may know that the unknowns commute, so we can choose a commutative ring. There are usually general grounds for believing that it is semisimple (B4, A7).

Now, a fairly complete structure theory exists for commutative, semisimple locally m-convex algebras (see Ref. 9, where the term locally m-convex is defined by Definition 2.1), which is sufficiently general to allow the unbounded spectra often required in physical problems. On the other hand, it would be most unfortunate if the algebra were really (which algebra? the whole point is that we do not know) merely locally convex, and not locally m-convex. We could not then do anything, even if we knew which algebra to choose. In other words, the idea here is to choose the most general structure which known pure mathematics enables us to handle and to ignore the possibility that this may be wrong on the grounds that the resulting situation would anyway be impossible to deal with.

In this spirit, consider the lowest-order complete unitarity[10] equations for the scattering of pseudoscalar "pions." Ignoring some physically important but mathematically merely confusing detail, these equations may be written (A8)

$$M - M' = -kMM', \tag{3}$$

$$M = -k \sum_{i=1,2,3} P_i(MM'), \tag{4}$$

where M represents the two-particle scattering amplitude, M' is a reduced amplitude obtained by removing contributions with certain singularities in the 1–2 channel, the propagators have been absorbed, and k is a pure imaginary constant. In this case, the multiplication is partly of Faltung type and partly pointwise (because of the δ function conserving 4-momentum). The P_i are all (topologically different, Ref. 10, Paper 3) permutations of the legs, and we have $P_i^2 = I$ for each i. [We follow, in general, the treatment of these equations given in Ref. 1, where careful references are given, proper sign conventions set up, etc. However, the present treatment improves on that of Ref. 1 in several respects. The question of the removal of singularities from the equations is carefully discussed in Ref. 10 (Paper 5, Appendix 3).]

Now strictly speaking (Ref. 10, loc. cit.), Eq. (3) is the *definition* of M'. Thus we can write meaningfully

$$M' = M/(1 - kM),$$

since otherwise M' would not be correctly defined by the Green's function analysis in Ref 10. Thus M and M' define a commutative ring. Suppose, according to our preliminary discussion, that this can be embedded into a complete, semi-simple locally m-convex algebra (B5). Then by Ref. 9, Proposition

[5] M. A. Krasnosel'skii, *Topological Methods in the Theory of Nonlinear Integral Equations* (The Macmillan Company, New York, 1964).
[6] J. G. Taylor, Proc. Roy. Soc. (London) (to be published).
[7] (a) J. G. Taylor, J. Math. Phys. **6**, 1148 (1965).
(b) J. G. Taylor, Rutgers University preprints:
"Topological degree for Non-Compact Mappings";
"On the Existence of Field Theory, I and II", cf. J. Math. Phys. **7**, 1720 (1966).
[8] J. Schauder, Studia Math. **2**, (1930).
[9] E. A. Michael, Am. Math. Soc. Memoirs. No. 11 (1952).
[10] J. G. Taylor, Nuovo Cimento Suppl. Pt. 1, 857 (1963).

8.1, we can get a functional representation (A6) which is an isomorphism. In other words, we can assume that the multiplication is pointwise and (3) and (4) then represent *all* Eqs. (2) for different χ.

We still have to deal with the extra terms on the right-hand side of (4). For this purpose, we must discuss involutions (A9). The natural one is TCP. Since we are working with the Fourier transforms of τ functions[11] rather than with the τ functions themselves, and since certain amputations have been performed,[10] TCP is not directly applicable. Nevertheless, one can show that there exists an involution related to TCP under which M is invariant.[12] The argument then proceeds exactly as in Ref. 1: on each point of the structure space (A10), i.e., essentially for each one of Eqs. (2), the symmetry property of M derived from TCP gives $\chi(M)$ real. Then the functions $\chi\{P_i(MM')\}$ must be $\chi(MM')$ multiplied by certain real functions (see Ref. 1 for details), and then Eqs. (2) have, by inspection, no solution other then the trivial one $M = M' = 0$.

The conclusion of this analysis is the following: Take the 2-cut approximation equations to the $\rho\phi^4$ pseudoscalar meson theory, developed by Taylor in Ref. 10 (Papers 3 and 5). These approximate equations are expected to give the scattering amplitude, at least up to the three-particle threshold. The process of discussing their solutions naturally gives rise to a certain commutative algebra with involution, for which the scattering amplitude M is a Hermitian element. If this algebra can be embedded into a semisimple locally m-convex *-algebra inducing the constructed involution, then the equations are without nontrivial solution. These equations are the pseudoscalar meson equivalent of the type of bootstrap equation proposed by Salam[13] in which all wave- and vertex-function renormalization constants vanish. The result suggests, therefore, that Salam-type bootstrap conditions are over restrictive.

The given analysis is considerably more general than that in Ref. 1, since there we assumed (rather than establishing) the existence of a suitable involution. We also used in Ref. 1 Banach algebras rather than the more general locally m-convex algebras of Ref. 9; this change removes some severe restrictions on the possible high-energy behavior of the scattering amplitude.

We now discuss a further and related method, applied in Ref. 2 to a number of bootstrap situations, but not fully described in that paper. This method is again at its best when the equations contain nothing but constants, unknowns, and (as usual) a multiplication operation.

In this method we consider the ring generated *algebraically* by the quantities appearing in the equation. Any solution must give rise to a representation of this ring. The ring structure is easiest to handle where the equations are polynomials. Suppose for the sake of example, we have two equations in two unknowns

$$p_1(x, y) = 0, \qquad p_2(x, y) = 0, \tag{5}$$

where the p's are polynomials with complex coefficients, say. However, the unknowns are supposed to be something perhaps quite complicated such as quantized fields (B6). Equations (5) could then be bootstraps for, say, a scalar meson interacting with a fermion via a Yukawa-type interaction, as discussed in Ref. 2, Sec. 7.

We may consider the polynomial domain $C[\theta_1, \theta_2]$ in two indeterminates (A11). Equations (5) can be regarded as relations on the ring $C[\theta_1, \theta_2]$, that is, they identify with the zero polynomial all polynomials having a factor p_1 or p_2. Thus, any solution of (5) can be regarded as a representation of the quotient ring (A11),

$$C[\theta_1, \theta_2]/(p_1, p_2).$$

In the physical example we mentioned, there is a physical requirement to the effect that this quotient ring be *not* semisimple; we have, in effect, a special

[11] H. Lehmann, K. Symanzik, and W. Zimmermann, Nuovo Cimento **25**, 425 (1955); K. Symanzik, CERN preprint (1961).

[12] We sketch the argument involved, since it has not appeared in print. We have to construct the involution and to show that M is invariant under it. Since the algebra is generated by M, it is sufficient to do this for polynomials in M. The ring anti-isomorphism is constructed simply by reversing the legs in the s channel. We are, of course, working with the complex field K, and the required anti-linearity in K will be the natural one. We are still free to fix a factor ± 1 in the transformation $M \to M^*$, and we do this precisely so as to have $M = M^*$. This is possible since $|M|$, regarded as a numerical function of four-momenta, in any case invariant under the ring anti-isomorphism (say, by field-theoretic crossing, see Ref. 10, p. 991) (even off-the-mass-shell, compare the continuation equation, the τ-function analog of Eq. 23) (p. 881, Ref. 10). Thus we also maintain $M^{**} = M$, as we must. We regard this involution as fixed before we embed the algebra of polynomials into a suitable complete locally m-convex algebra, (i.e., by taking an appropriate uniform structure on the polynomial algebra), since the completion of the algebra of polynomials will depend *a priori* on the involution. The connection with TCP is now logically redundant, but can be seen easily enough by writing down the expression for M as the Fourier transform of the vacuum expectation value of the time-ordered product of fields. (We are indebted to Dr. J. G. Taylor for pointing out the difficulties which arise when one tries to establish a *direct* connection between TCP and the involution.) Finally, we note that this is not quite the same involution as that used in Appendix 1 of Ref. 1.

[13] A. Salam, Nuovo Cimento **25**, 224 (1962).

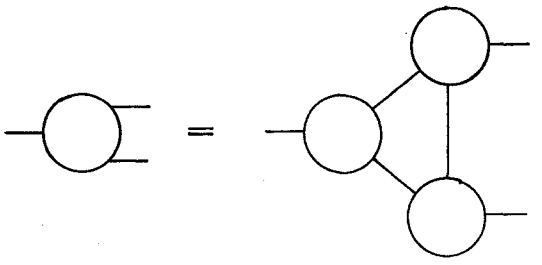

FIG. 1. Scalar meson bootstrap.

situation contradicting the remarks made in connection with the previous example. This special situation arises because Eqs. (5) are to be bootstraps, so in particular must determine enough degrees of freedom to describe a (quantized-field) particle. In a semisimple ring, they would only have a finite number, which is certainly not enough. One can show by standard arguments based on the ideal theory of commutative rings[4] that, if neither of the polynomials has a double factor, the ring will indeed be semisimple. This is the case for all the situations analyzed in Ref. 2.

It may easily happen, however, that the values of the constants in the equations *do* permit solutions in rings which are not semisimple. In this case, one has not made very much progress, but at least one has a clue at which type of operator to look at: subdiagonal matrices or Volterra kernels, for instance.

This method, then, is more general than the previous one, but gives less information. Had we applied to the previous one, we would have been much firmer in our conclusion that there is no physically meaningful solution to the bootstraps (5)—but this would have been at the price of *assuming* semisimplicity, whereas we can now see whether or not the assumption would have been reasonable.

The so-called axioms of field theory (e.g., Ref. 14, p. 52) are sufficiently general to allow nonsymmetric operators; though since a single symmetric operator generates[15] (B7) a semisimple algebra, this would necessitate the use of complex-valued test functions all the time.

Consider in more detail what happens in the semisimple case. The equations themselves give information only about each simple direct summand, since other ring products vanish identically. Each direct summand is in all the usual cases a domain of integrity, that is, we can cancel factors. Then the *only* solutions are the ones obtained by "high-school algebra". For instance, the field equation for a scalar meson with n–tic interaction

$$(\Box^2 + m^2)\phi = g\phi^n$$

gives rise[2] to the bootstrap

$$\delta m^2\phi = g\phi^n;$$

and since the roots of $\theta(1 - \mu\theta^n) = 0$ are always distinct, the quotient ring is always semisimple. Hence we can cancel factors and obtain $\phi = \text{const}$. This can give no particle creation or annihilation.

Natural approximations (which do not damage the algebraic structure, cf. note A8) then give rise to the Green's function equation (we take $n = 3$ for simplicity) (Ref. 10, Paper 6) (see Fig. 1).

This is no longer an equation on a ring. Yet one can go back to the algebraic structure of the operator equations. Hence we avoid the paradox mentioned in note A8. Every significant solution of this equation corresponds to a significant solution of the operator equation. The identity operator cannot correspond to a Green's function; hence we have only the zero solution [as has been shown by other methods—topological methods[7(a)] and direct algebraic methods of a special type[16]]. This is an example of the way a well-defined Green's function equation obtained from a poorly defined operator equation can nevertheless be discussed by transferring the structure of the operator equation.

We still have nothing to say about bootstraps with derivative coupling. It seems clear that, if an algebraic argument is possible, it must be of the homological type hinted at in the notes. We hope to return to this topic elsewhere.

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APPENDIX A

A1. A *ring* is a set of elements $a, b, c, \cdots$ for which are defined an addition and a multiplication satisfying the usual laws of high-school algebra:

$$a(b \pm c) = ab \pm ac, \qquad (ab)c = a(bc).$$

A *commutative* ring is a ring whose elements in addition satisfy $ab = ba$ for each pair (a, b) of elements. An *algebra* is a ring equipped with a set of scalars $\lambda, \mu, \cdots$ such that

[14] R. Jost, *General Field Theory* (American Mathematical Society, Providence, Rhode Island, 1965).

[15] M. M. Broido, Proc. Cambridge Phil. Soc. **62**, 209 (1966); M. M. Broido, *ibid.* (to be published).

[16] M. M. Broido, Ph.D. thesis, Cambridge University (1965).

$$\lambda(a \pm b) = \lambda a \pm \lambda b$$

and commuting with all elements a, b, $\cdots$. We assume without further comment that all algebras are *over the complex field*, i.e., the scalars λ, μ, $\cdots$ can be any complex numbers.

A2. That is, each term is of the form $px^m y^n \cdots$, where p is given and x, y, $\cdots$, are unknowns. We do not concern ourselves with the detailed relationship between the number of equations and the number of unknowns.

A3. That is, essentially, the methods by which a set of polynomial equations in several unknowns may be reduced to a series of equations each with only one unknown.

A4. A *homomorphism* of a ring into another ring is a mapping which preserves sums and products. A *character* of a ring is, for our purposes, a homomorphism into the field of complex numbers.

A5. Suppose they are indexed by an index α. There are "sufficiently many" characters χ_α if, given that $\chi_\alpha(a) = 0$ for all α, we can conclude that $a = 0$.

A6. A *functional representation* of a ring is a homomorphism (see A4 above) into a ring of functions; because the multiplication is pointwise, we are then given many characters explicitly.

A7. Roughly speaking, a ring is *simple* if every nontrivial homomorphism is an isomorphism. A ring is *semisimple* if it is the direct sum, product, integral, etc., of simple rings. Again, roughly speaking, anything to do with fermions is unlikely to give rise a semisimple ring because of the relations $q^2 = \bar{q}^2 = 0$ arising from the spin-statistics theorem. [See Ref. 2, Sec. 7.2(d), for difficulties arising from this circumstance.] In fact, the algebra generated by polynomials in q, say, is always a radical algebra (isomorphic as a vector space to the base field, with all ring-products zero). Of course, if one embeds q and $\bar{q}$ into a very large (say, irreducible) operator algebra, this is always semisimple, but such a large algebra is very difficult to handle.

A8. The essence of the method, in fact, is the recognition that the equations can be written in this "multiplicative" form. Such a form is vital to our arguments, and care must be taken not to destroy it by approximations. For instance, a certain set of two-body bootstrap equations[17] can be expressed in terms of Feynman graphs in the form

$$\Gamma = \int \Gamma S S \Gamma, \qquad \text{(a1)}$$

which reduces in the high-energy limit to

$$\Gamma(p) = \int_p^\infty \Gamma^3(h)\, dh. \qquad \text{(a2)}$$

By the method presented in the text, one argues (we omit the details) that (a1) has no solutions. Nevertheless, (a2) clearly does have solutions. The point is that the ring-multiplication in (a1) has been destroyed by passing to (a2), and our method no longer applies. One can look at it another way: a solution of (a2) cannot necessarily be continued out of the high-energy region to give a solution to the structurally different equation (a1). (We are grateful to Dr. L. Castillejo for drawing our attention to this argument.)

A9. An involution is a mapping of an algebra onto itself satisfying

$$(\lambda a + \mu b)^* = \overline{\lambda} a^* + \overline{\mu} b^*, \qquad (ab)^* = b^* a^*$$

(examples: Hermitian conjugation for matrices; TCP for quantum field operators).

A10. The functions of the functional representation A6 are functions on this space.

A11. See Ref. 4, Vol. 1. The indeterminate are essentially "meaningless" symbols which commute with one another, and $C[\theta_1, \theta_2]$ is the set of all polynomials with complex coefficients in the two indeterminates θ_1, θ_2.

APPENDIX B

B1. There is an important case, which we use in the sequel, where this reconstruction can be carried out explicitly. This is the case of a commutative, semisimple, complete locally m-convex algebra [the latter term is defined in Ref. 9, Definition 2.1, and the assertion is a direct consequence of Lemma 7.3(d) and Proposition 8.1 of Ref. 9].

The theory of categories provides a suitable general language in which to discuss these matters. For instance, the class of locally convex algebras over the complex field K, with morphisms those continuous ring-homomorphisms which are also homomorphisms of K-algebras, form a category $\mathcal{A}$. The question of whether such a category can be adequately "represented" by, say, a subcategory $\mathcal{A}_1$ consisting of operators in some special type of locally convex space, is simply the question of whether $\mathcal{A}$ is equivalent to its full subcategory $\mathcal{A}_1$. This is the case, for instance, with semisimple symmetric Banach *-algebras and uniformly closed *-algebras of operators on Hilbert spaces. Most of the arguments in the present paper can be formulated in terms of those notions, though we have not yet

[17] R. Brout and F. Englert, Bull. Am. Phys. Soc. 11, 21 (1966).

found it worthwhile to do so. A version of such a categorical discussion appears already in Ref. 1, Appendix C, in a very disguised form.

B2. Such situations are doubtless execrable to most mathematicians; but they arise in practice, and must somehow be dealt with.

B3. It may be a more complicated algebraic structure. In what sort of category should we look? The usual mathematical methodology does not seem to provide any guide.

B4. The reasons for this are usually of a physical nature; see note A7.

B5. Since M' is a function of M, this is essentially an assumption to the effect that a certain *single* operator generates a locally m-convex algebra, rather than a more general locally convex algebra. One may inquire under what conditions this holds. It turns out[18] that there is a very large class of spaces on which *every* continuous linear operator generates in a natural way a locally m-convex algebra, although cases where two *commuting* operators do not do so can be constructed easily. This class of spaces appears to contain all projective limits of Hilbert spaces (hence, in particular, all nuclear spaces) and many spaces possessing natural embeddings into their duals.

B6. A quantized field is essentially a distribution on one of the usual nuclear spaces of test-functions, taking values in an appropriate operator algebra. Such distributions do not, in general, allow a multiplication of the type postulated (i.e., associative, commutative, and distributive); this is one of the central problems of quantum field theory. We assume tacitly that, for our fields, such a multiplication can be defined. There are powerful physical arguments behind this assumption, discussed in detail in Ref. 2, Sec. 7, and references quoted there.

B7. It is practically obvious that any reasonable commutative algebra generated by a symmetric operator A on a Hilbert space H has a natural structure as a *-algebra with A Hermitian, since A has real spectrum in H. Then for $\phi \in H$, the functional $B \to (\phi, B\phi)$ is a positive functional on the algebra. In the particular case of the algebras constructed in Ref. 15, the semisimplicity follows directly from Ref. 9, Proposition 7.4.

[18] M. M. Broido (to be published).

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Two-Meson Solution of the Charged Scalar Static Model with Bound States

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(Received 11 April 1966)

A two-meson solution of the charged scalar static model is constructed for the case in which the coupling is sufficient to produce bound states. This is done by taking the solution given previously for the case in which bound states are absent and increasing the coupling. As usual, bound states appear as poles in scattering amplitudes. However, since one of the mesons in the three-body states can bind to the source, bound-state meson scattering channels also appear. The new amplitudes relating to bound-state meson scattering are obtained, and their unphysical singularities are examined. The enlarged scattering matrix is unitary.

I. INTRODUCTION

A SOLUTION of the charged scalar static model was recently given in which the scattering amplitude is crossing symmetric and satisfies two- and three-particle unitarity.[1] (We refer to Ref. 1 as paper I.) Like the usual one-meson solution, the new two-meson solution has $\pi^+ - p$ and $\pi^- - n$ bound states when the coupling is sufficiently strong. However, in the two-meson solution, the bound states do not manifest themselves solely as poles of the transition amplitudes. Here, they also occur in bound-state meson intermediate states. Such states arise automatically due to the possibility that one of the mesons in a three-body intermediate state may bind to the source. In this paper, we re-examine the two-meson solution given in I in the presence

[1] J. B. Bronzan, J. Math. Phys. 7, 1351 (1966).

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of bound states. We obtain all the transition amplitudes in the problem, including the three new ones which involve the bound-state meson channels. The unphysical singularities of the new amplitudes and the unitarity of the scattering matrix are examined.

All of the results we obtain are contained implicitly in I. (We refer the reader to I for a review of the elementary properties of the charged scalar static model and for a discussion of results introduced in the present paper without derivation.) Our method is to take the two-meson amplitudes given in I and increase the coupling until bound states occur. We then find that the amplitudes have new poles and cuts, and we thereby determine the parameters of the bound states and the new amplitudes involving bound-state meson scattering states. For example, the two-meson scattering amplitude for $\pi^+ + p \to \pi^+ + p$ develops a pole corresponding to the bound state B^{++}, and the crossed-scattering amplitude for $\pi^- + p \to \pi^- + p$ develops a cut due to the intermediate state $\pi^+ + B^-$. The discontinuity across this cut must be proportional to the square of the modulus of the amplitude for $\pi^- + p \to \pi^+ + B^-$. This point can be checked in the following manner. We note that, in the presence of bound states, the production amplitude for $\pi^- + p \to \pi^+ + \pi^- + n$ develops a pole in the energy of the outgoing π^- corresponding to the sequence

$$\begin{aligned} \pi^- + p &\to \pi^+ + B^- \\ &\quad\;\; \big\vert\!\to \pi^- + n. \end{aligned}$$

From the residue of this pole, we determine the amplitude for $\pi^- + p \to \pi^+ + B^-$. In a similar fashion, we can read off all the other amplitudes involving bound-state meson channels without solving new dispersion equations. We carry out this program in the following sections.

The foregoing outline suggests some of the results we obtain. First, the bound-state meson channels arise from the coalescence of a meson in a three-particle state with the source. Accordingly, we expect the solutions to involve channels with one meson and a bound state, but not two mesons and a bound state. Second, the bound states appearing in the bound-state meson scattering states have the mass m_B and coupling constant g_B determined by the auxiliary one-meson solution M_+. In paper I, this solution was used as a final-state scattering amplitude, and it therefore governs the properties of a bound state occurring as a coalescence in a three-particle state. On the other hand, the bound-state pole of the two-meson scattering amplitude T_+ occurs at a lower mass M_B and has a different coupling constant G_B. The shift is a consequence of the attractive forces which are absent in M_+ but included in T_+. This discrepancy is not to be regretted altogether, since it provides a measure of the influence of three-particle states on bound-state parameters in this model. It follows from these remarks that there must exist a limited range of couplings for which T_+ has developed a bound-state pole, but no bound state cuts have as yet appeared. Reference 2 provides a numerical study of the range of couplings for which T_+, but not M_+, has a bound state.

The third result we anticipate is that our scattering matrix continues to be unitary after the new amplitudes involving bound states have developed. Roughly, this is because unitarity, which was established to be satisfied in I, is not a function of the coupling constant. It follows that the new amplitudes have the discontinuities across physical cuts dictated by unitarity. On the other hand, the unphysical singularities of these amplitudes are not expected to be completely accurate. Two of the three new amplitudes are obtained as the residues of appropriate pole terms in production and six-point amplitudes. It was pointed out in I that the production and six-point amplitudes are not crossing symmetric, even though the scattering amplitude is. Since the crossed singularities of the production and six-point amplitudes become the unphysical singularities of the bound-state meson amplitudes, we expect that the latter has unphysical singularities which are partly incorrect.

II. ONE-MESON AMPLITUDES WITH BOUND STATES

In paper I, we introduced the one-meson amplitudes $M_+(\omega)$ and $M_-(\omega)[=M_+(-\omega - i\epsilon)]$ referring to $\pi^+ - p$ and $\pi^- - p$ elastic scattering. We also defined the Omnes functions $\Delta_\pm(z)$ as

$$\Delta_\pm(z) = \exp\left[\frac{z}{\pi}\int_\mu^\infty \frac{d\omega_1\ \delta_\pm(\omega_1)}{\omega_1(\omega_1 - z)}\right]. \tag{1}$$

Here, $\delta_\pm(\omega)$ are the real phase shifts obtained in the one-meson approximation. When the meson-source coupling constant g is so small that no $\pi^+ - p$ bound state occurs, we can represent $M_+(\omega)$ as

$$M_+(\omega) = (g^2/\omega)\ \Delta_+(\omega + i\epsilon)\ \Delta_-(-\omega). \tag{2}$$

We now increase g so that $M_+(\omega)$ develops a B^{++} bound-state pole. If we take Eq. (1) and continue in g, we find that the continuation of Δ_+, Δ_+^c, de-

[2] J. B. Bronzan and R. W. Brown, Ann. Phys. (N. Y.) 39, 335 (1966).

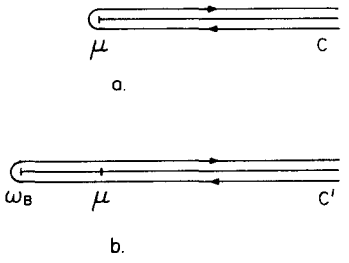


FIG. 1. Contours in the complex ω_1 plane for the evaluation of Δ_+^c.

velops the pole too. Accordingly, Eq. (2) remains valid when there is a bound state if we replace Δ_+ by Δ_+^c. We arrange our notation as follows. We let Δ_+ denote the integral in Eq. (1) both when a bound state is absent and when it is present. When a bound state develops, $\delta_+(\mu)$ changes discontinuously from 0 to π. Corresponding to this, Δ_+ suddenly develops a pole at $z = \mu$. On the other hand, Δ_+ passes smoothly into its continuation Δ_+^c as the bound state develops.

Let us now obtain Δ_+^c. We note that, when no bound state is present, we may write Δ_+ as

$$\Delta_+(z) = \exp\left[\frac{z}{2i\pi}\int_C \frac{d\omega_1 \ln M_+(\omega_1)}{\omega_1(\omega_1 - z)}\right], \qquad (3)$$

where C is the contour shown in Fig. 1(a). Now, as we let M_+ develop a bound-state pole at $\omega_B = m_B - m$ (m is the mass of the source), $\ln M_+(\omega)$ develops a new cut which deforms the contour as shown in Fig. 1(b). The discontinuity across the anomalous cut is $2\pi i$, so, writing the contour integral as an integral of the discontinuity across the cut, we find

$$\Delta_+^c(z) = \Delta_+(z)\exp\left[z\int_{\omega_B}^{\mu}\frac{d\omega_1}{\omega_1(\omega_1 - z)}\right] = \frac{\omega_B(z-\mu)}{\mu(z-\omega_B)}\Delta_+(z). \qquad (4)$$

Note that the factor $(z - \mu)$ removes the pole which has developed in $\Delta_+(z)$ at threshold, while the factor $(z - \omega_B)$ inserts the bound-state pole. When a bound state is present, Eq. (2) becomes

$$M_+(\omega) = \frac{g^2}{\omega}\Delta_+^c(\omega + i\epsilon)\,\Delta_-(-\omega) = \frac{g^2\omega_B(\omega-\mu)}{\mu(\omega-\omega_B)\omega}\Delta_+(\omega + i\epsilon)\,\Delta_-(-\omega). \qquad (5)$$

From this equation, we can obtain a formula for g_B, the bound-state-source-meson coupling constant in the one-meson approximation. Examining the pole residues at $\omega = \omega_B$, we find

$$g_B^2/g^2 = \mu^{-1}(\mu - \omega_B)\,\Delta_+(\omega_B)\,\Delta_-(-\omega_B). \qquad (6)$$

III. THE TWO-MESON SCATTERING AMPLITUDES WITH BOUND STATES

In paper I, we obtained the two-meson scattering amplitude $T_+(\omega) = T_-(-\omega)$,

$$T_+(\omega) = \frac{g^2\omega^{-1}}{\alpha(\omega) + [1 - \omega C(\omega)][1 + \omega C(\omega)]^{-1}},$$

$$\alpha(\omega) = -\frac{2\omega g^2}{\pi}\int_\mu^\infty \frac{d\omega_1\, k_1 u^2(\omega_1)}{4\pi\omega_1(\omega_1^2 - \omega^2)},$$

$$C(\omega) = \frac{1}{\pi}\int_{2\mu}^\infty \frac{d\omega_1}{\omega_1}\left[\frac{\rho_+(\omega_1)}{\omega_1 - \omega - i\epsilon} + \frac{\rho_-(\omega_1)}{\omega_1 + \omega + i\epsilon}\right],$$

$$\rho_+(\omega) = \frac{\omega^3}{16\pi^3}\left|\frac{M_-(\omega)}{\Delta_-(\omega)}\right|^2\int_\mu^{\omega-\mu} d\omega_1\, k_1 k_{-1} u^2(\omega_1)u^2(\omega_{-1}) \times |\Delta_-(\omega_1 + i\epsilon)\,\Delta_-(\omega_{-1} + i\epsilon)(\omega_1\omega_{-1})^{-1}|^2, \qquad (7)$$

$$\rho_-(\omega) = \frac{\omega}{8\pi^3}\left|\frac{M_+(\omega)}{\Delta_+(\omega)}\right|^2\int_\mu^{\omega-\mu} d\omega_1\, k_1 k_{-1} u^2(\omega_1)u^2(\omega_{-1}) \times |\Delta_+(\omega_1 + i\epsilon)\,\Delta_-(\omega_{-1} + i\epsilon)(\omega_{-1})^{-1}|^2,$$

where $\omega_{-1} = \omega - \omega_1$, $k_{-1} = (\omega_{-1} - \mu^2)^{\frac{1}{2}}$, and $u^2(\omega)$ is the cutoff function. As we increase g, T_+ develops a bound-state pole. Because of the inclusion of production through the integral $C(\omega)$, this pole develops for smaller values of g than does the pole in M_+. Correspondingly, it occurs at a slightly different energy $\tilde{\omega}_B = M_B - m$ and with a different coupling G_B. For couplings such that M_+ has not yet developed a bound state, Eq. (7) is correct as it stands. However, when g is sufficiently large for M_+ to have a bound-state pole, the dispersion representation of $C(\omega)$ is modified, and this modification represents the introduction of $\pi^+ - B^-$ intermediate states into the dispersion relation for T_+. We note that ρ_+ is defined in terms of objects which do not develop new singularities as M_+ develops a pole. Consequently, ρ_+ is still given by the integral in Eq. (7) when M_+ has a bound state. On the other hand, ρ_- is no longer given by the integral in Eq. (7) after M_+ develops a bound state. Therefore, our task is to continue ρ_- in g into the bound-state region.[3]

We note that ρ_- may be written in the following form when no bound states are present:

[3] In the remainder of this paper, we take "bound-state region" to mean the range of couplings for which both T_+ and M_+ exhibit bound states and, therefore, for which T_+ has a cut due to bound-state meson intermediate states.

$$\rho_-(\omega) = \frac{\omega}{8\pi^3}\left|\frac{g^2}{\omega}\Delta_-(-\omega)\right|^2 \int_\mu^{\omega-\mu} d\omega_1\, k_1 k_{-1} u^2(\omega_1) u^2(\omega_{-1})\, |\omega_1 M_+(\omega_1) M_-(\omega_{-1})[g^2\,\Delta_-(-\omega_1) g^2\,\Delta_+(-\omega_{-1})]^{-1}|^2$$
$$= -\frac{\Delta_-^2(-\omega)}{2\pi g^4 \omega}\int_\mu^{\omega-\mu} \frac{d\omega_1\,\omega_1^2}{\Delta_-^2(-\omega_1)\,\Delta_+^2(-\omega_{-1})}\,[M_+(\omega_1+i\epsilon) - M_+(\omega_1 - i\epsilon)][M_-(\omega_{-1}+i\epsilon) - M_-(\omega_{-1}-i\epsilon)]. \tag{8}$$

In obtaining the second form, we have recognized that

$$M_\pm(\omega + i\epsilon) - M_\pm(\omega - i\epsilon) = [iku^2(\omega)/2\pi]\,|M_\pm(\omega)|^2$$

and that the other quantities under the absolute value signs are real for $\omega > 2\mu$. Thus,

$$\rho_-(\omega) = -[\Delta_-^2(-\omega)/2\pi g^4\omega][I_+ - I_-],$$
$$I_\pm = \int_\mu^{\omega-\mu} \frac{d\omega_1\,\omega_1^2[M_+(\omega_1+i\epsilon) - M_+(\omega_1 - i\epsilon)]M_-(\omega_{-1}\pm i\epsilon)}{\Delta_-^2(-\omega_1)\,\Delta_+^2(-\omega_{-1})}$$
$$= \int_{C_\pm} \frac{d\omega_1\,\omega_1^2 M_+(\omega_1) M_-(\omega_{-1}\pm i\epsilon)}{\Delta_-^2(-\omega_1)\,\Delta_+^2(-\omega_{-1})}. \tag{9}$$

C_+ is the contour shown in Fig. 2(a); a similar contour applies for C_-. $I_\pm$ are now suitable for continuation in g. As M_+ develops a pole, C_+ is deformed into C_+' as shown in Fig. 2(b). We separate off the contribution of the pole to obtain

$$I_\pm^c = \frac{2\pi i g_B^2 \omega_B^2 M_-(\omega - \omega_B \pm i\epsilon)}{\Delta_-^2(-\omega_B)\,\Delta_+^{c\,2}(\omega_B - \omega)}$$
$$+ \int_{C_\pm} \frac{d\omega_1\,\omega_1^2 M_+(\omega_1) M_-(\omega_{-1}\pm i\epsilon)}{\Delta_-^2(-\omega_1)\,\Delta_+^{c\,2}(-\omega_{-1})}, \tag{10}$$

and therefore,

$$\rho_-^c(\omega) = \rho_-^T(\omega) + \rho_-^B(\omega),$$
$$\rho_-^T(\omega) = \frac{\omega(\omega-\omega_B)^2}{8\pi^3(\omega-\mu)^2}\left|\frac{M_+(\omega)}{\Delta_+(\omega)}\right|^2$$
$$\times \int_\mu^{\omega-\mu} d\omega_1\, k_1 k_{-1} u^2(\omega_1) u^2(\omega_{-1})$$
$$\times |[(\omega_1-\mu)/(\omega_1-\omega_B)\omega_{-1}]\,\Delta_+(\omega_1)\,\Delta_-(\omega_{-1})|^2,$$
$$\rho_-^B(\omega) = \frac{g_B^2\mu^4\omega^3\bar{\omega}^2 k u^2(\bar{\omega})\,|M_-(\bar{\omega})|^2}{2\pi g^8\omega_B^2(\omega-\mu)^2(\bar{\omega}+\mu)^2\,\Delta_-^2(-\omega_B)\,\Delta_+^2(-\bar{\omega})}$$
$$\times \left|\frac{M_+(\omega)}{\Delta_+(\omega)}\right|^2. \tag{11}$$

Here $\bar{\omega} = \omega - \omega_B$. ρ_-^T is obtained from ρ_- by replacing Δ_+ by Δ_+^c everywhere it appears; consequently, it represents the contribution to T_+ of three-particle states $n\pi^+\pi^-$. ρ_-^B is a new term, with threshold $\mu + \omega_B < 2\mu$. It represents the $\pi^+ B^-$ intermediate state, and we expect that the integral over ρ_-^c must be extended to the threshold of ρ_-^B. Therefore, subject to later verification, we find that, in the bound-state region,

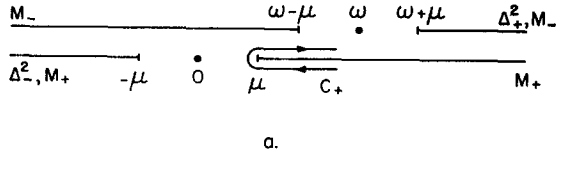
$$T_+(\omega) = \frac{g^2\omega^{-1}}{\alpha(\omega) + [1-\omega C(\omega)][1+\omega C(\omega)]^{-1}},$$
$$C(\omega) = \frac{1}{\pi}\int_{\mu+\omega_B}^\infty \frac{d\omega_1\,\rho_-^B(\omega_1)}{\omega_1(\omega_1+\omega+i\epsilon)}$$
$$+ \frac{1}{\pi}\int_{2\mu}^\infty \frac{d\omega_1}{\omega_1}\left[\frac{\rho_+(\omega_1)}{\omega_1-\omega-i\epsilon} + \frac{\rho_-^T(\omega_1)}{\omega_1+\omega+i\epsilon}\right]. \tag{12}$$

IV. THE AMPLITUDE FOR $B^- + \pi^+ \to p + \pi^-$

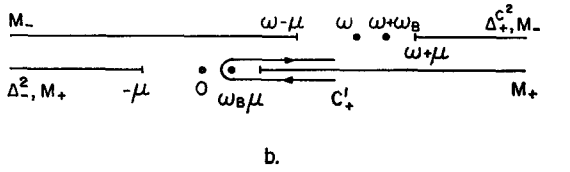
Equation (12) was obtained by a straightforward continuation in g of the formula derived in I. We now want to verify that it is a solution of the dispersion relation for $T_+(\omega)$ in the two-meson approximation when bound states are present. To this end, we define the amplitude for the transition $B^- + \pi^+ \to p + \pi^-$ as

$$H(\omega) = [(2\omega\Omega)^{\frac{1}{2}}/u(\omega)]\langle \pi_k^- p \text{ out } |j^\dagger(0)|\, B^-\rangle. \tag{13}$$

The dispersion relation for $T_+(\omega)$ in the presence of bound states is



a.



b.

FIG. 2. Contours in the complex ω_1 plane for the evaluation of I_+. The endpoints of C_+ may be taken to be any points between $\omega - \mu$ and ω; the dependencies of I_+ and I_- on the endpoints cancel in ρ_-. The cuts are labeled by the factors in the integrand of I_+ which give rise to them.

$$T_+(\omega) = \frac{g^2}{\omega} - \frac{G_B^2}{\omega - \tilde{\omega}_B} + \frac{1}{\pi}\int_\mu^\infty \frac{d\omega_1\, k_1 u^2(\omega_1)}{4\pi}\left[\frac{|T_+(\omega_1)|^2}{\omega_1 - \omega - i\epsilon} + \frac{|T_-(\omega_1)|^2}{\omega_1 + \omega + i\epsilon} + \frac{|H(\omega_1 + \omega_B)|^2}{\omega_1 + \omega_B + \omega + i\epsilon}\right]$$
$$+ \frac{1}{\pi^2}\int_\mu^\infty\int_\mu^\infty \frac{d\omega_1\, d\omega_2\, k_1 k_2 u^2(\omega_1)u^2(\omega_2)}{16\pi^2}\left[\frac{|P_+(\omega_1, \omega_2)|^2}{\omega_1 + \omega_2 - \omega - i\epsilon} + \frac{|P_-(\omega_1, \omega_2)|^2}{\omega_1 + \omega_2 + \omega + i\epsilon}\right]. \quad (14)$$

As in I, T_- is given by the crossing relation $T_-(\omega) = T_+(-\omega - i\epsilon)$. In order to verify that Eq. (12) satisfies Eq. (14), we need H and the production amplitudes P_+ and P_-. P_+ and P_- are obtained from I by continuation in g. This does not affect P_+, so P_+ is still given by Eq. (44I).[4] For P_-, the continuation amounts to replacing Δ_+ by Δ_+^c in Eq. (40I). We then obtain

$$P_+(\omega_1, \omega_2) = \frac{g(\omega_1 + \omega_2)}{(2)^{\frac{1}{2}}\omega_1\omega_2}\left[T_+(\omega_1 + \omega_2) - M_-(\omega_1 + \omega_2)\right]\frac{\Delta_-(\omega_1 + i\epsilon)\,\Delta_-(\omega_2 + i\epsilon)}{\Delta_-(\omega_1 + \omega_2 + i\epsilon)},$$

$$P_-(\omega_1, \omega_2) = \frac{g}{\omega_1}\left[T_-(\omega_1 + \omega_2) - M_+(\omega_1 + \omega_2)\right]\frac{(\omega_2 - \mu)(\omega_1 + \omega_2 - \omega_B)}{(\omega_1 + \omega_2 - \mu)(\omega_2 - \omega_B)}$$
$$\times \Delta_-(\omega_1 + i\epsilon)\,\Delta_+(\omega_2 + i\epsilon)[\Delta_+(\omega_1 + \omega_2 + i\epsilon)]^{-1}, \quad (15)$$

for the production amplitudes in the bound-state region.

$H(\omega)$ is obtained by noting that the dispersion relation for Q_- [Q_- is related to P_- in I] becomes

$$Q_-(\omega_1, \omega_2) = \frac{g}{\omega_1 - \omega_2 - i\epsilon}\left[T_-^*(\omega_1) - M_+^*(\omega_1)\right] - \frac{g_B H^*(\omega_1)}{\omega_B - \omega_2 - i\epsilon}$$
$$+ \frac{1}{\pi}\int_\mu^\infty d\omega'\left[\frac{e^{-i\delta_+(\omega')}\sin\delta_+(\omega')Q_-(\omega_1, \omega' + i\epsilon)}{\omega' - \omega_2 - i\epsilon} + \frac{e^{-i\delta_-(\omega')}\sin\delta_-(\omega')Q_-(\omega_1, \omega_1 - \omega' - i\epsilon)}{\omega' - \omega_1 + \omega_2 + i\epsilon}\right] \quad (16)$$

in the presence of a bound state. Equation (16) has the status of being the dynamical equation which determines Q_- and P_- in our calculation. We see that, when a $\pi^- n$ bound state is present, a new pole occurs at $\omega_2 = \omega_B$. The residue of this pole is related to $H(\omega)$,

$$H^*(\omega_1) = \frac{1}{g_B}\lim_{\omega_2 \to \omega_B}(\omega_2 - \omega_B)Q_-(\omega_1, \omega_2). \quad (17)$$

On the other hand, Eq. (40I) implies that, when bound states are present, Q_- must be given by the expression

$$Q_-(\omega_1, \omega_2) = -\frac{g}{\omega_1 - \omega_2 - i\epsilon}\left[T_-^*(\omega_1) - M_+^*(\omega_1)\right]\frac{(\omega_2 - \mu)(\omega_1 - \omega_B)}{(\omega_1 - \mu)(\omega_2 - \omega_B)}$$
$$\times \Delta_+(\omega_2 + i\epsilon)\,\Delta_-(\omega_1 - \omega_2 - i\epsilon)[\Delta_+(\omega_1 - i\epsilon)]^{-1}. \quad (18)$$

Thus

$$H(\omega) = \frac{g(\omega_B - \mu)}{g_B(\omega - \mu)}\left[T_-(\omega) - M_+(\omega)\right]$$
$$\times \frac{\Delta_+(\omega_B)\,\Delta_-(\omega - \omega_B + i\epsilon)}{\Delta_+(\omega + i\epsilon)}. \quad (19)$$

With the aid of Eqs. (15) and (19), one can verify that Eq. (12) satisfies Eq. (14). In addition, Eq. (18) is readily verified to be a solution of Eq. (16).

V. THE OTHER AMPLITUDES FOR SCATTERING FROM THE BOUND STATE

In order to complete our discussion, we want to verify that our scattering matrix is unitary. For that purpose, we need the two amplitudes $J(\omega_1, \omega_2)$ and $K(\omega)$,

$$J(\omega_1, \omega_2) = [(2\omega_1\Omega 2\omega_2\Omega)^{\frac{1}{2}}/u(\omega_1)u(\omega_2)]$$
$$\times \langle \pi_{k_1}^+\pi_{k_2}^- n \text{ out } |j^\dagger(0)|\, B^-\rangle,$$
$$K(\omega) = [(2\omega\Omega)^{\frac{1}{2}}/u(\omega)]\langle \pi_k^+ B^- \text{ out } |j^\dagger(0)|\, B^-\rangle. \quad (20)$$

These amplitudes refer to $\pi^+ + B^- \to \pi^+ + \pi^- + n$ and $\pi^+ + B^- \to \pi^+ + B^-$, and they are connected by unitarity to H, P_-, and T_-. The amplitude J is obtained by a limiting procedure on the six-point amplitude R_-, which was obtained in paper I. In the presence of a bound-state, R_- satisfies the dispersion relation,

[4] The symbol "I" indicates that an equation in Ref. 1 is specified.

$$R_-(\omega_1, \omega_2, \omega_3) = \frac{gP^*_-(\omega_3, \omega_2)}{\omega_2 + \omega_3 - \omega_1 - i\epsilon} - \frac{g_B J^*(\omega_3, \omega_2)}{\omega_B - \omega_1 - i\epsilon}$$
$$+ \frac{1}{\pi}\int_\mu^\infty d\omega' \left[\frac{e^{-i\delta_+(\omega')}\sin\delta_+(\omega')R_-(\omega' + i\epsilon, \omega_2, \omega_3)}{\omega' - \omega_1 - i\epsilon} + \frac{e^{-i\delta_-(\omega')}\sin\delta_-(\omega')R_-(\omega_2 + \omega_3 - \omega' - i\epsilon, \omega_2, \omega_3)}{\omega' - \omega_2 - \omega_3 + \omega_1 + i\epsilon}\right]. \tag{21}$$

Therefore,

$$J^*(\omega_3, \omega_2) = \frac{1}{g_B}\lim_{\omega_1 \to \omega_B}(\omega_1 - \omega_B)R_-(\omega_1, \omega_2, \omega_3). \tag{22}$$

On the other hand, in the presence of a bound state, we find from Eq. (55I) the relation

$$R_-(\omega_1, \omega_2, \omega_3) = \frac{g^2[T^*_-(\omega_2 + \omega_3) - M^*_+(\omega_2 + \omega_3)](\omega_1 - \mu)(\omega_2 - \mu)}{\omega_3(\omega_2 + \omega_3 - \omega_1)(\omega_2 + \omega_3 - \mu)^2(\omega_1 - \omega_B)(\omega_2 - \omega_B)}$$
$$\times (\omega_2 + \omega_3 - \omega_B)^2 \frac{\Delta_-(\omega_3 - i\epsilon)\,\Delta_-(\omega_2 + \omega_3 - \omega_1 - i\epsilon)\,\Delta_+(\omega_1 + i\epsilon)\,\Delta_+(\omega_2 - i\epsilon)}{[\Delta_+(\omega_2 + \omega_3 - i\epsilon)]^2}. \tag{23}$$

We therefore find

$$J(\omega_1, \omega_2) = \frac{g^2[T_-(\omega_1 + \omega_2) - M_+(\omega_1 + \omega_2)](\omega_2 - \mu)(\omega_B - \mu)}{g_B\omega_1(\omega_1 + \omega_2 - \mu)^2(\omega_2 - \omega_B)}$$
$$\times (\omega_1 + \omega_2 - \omega_B)\frac{\Delta_+(\omega_B)\,\Delta_-(\omega_1 + i\epsilon)\,\Delta_-(\omega_1 + \omega_2 - \omega_B + i\epsilon)\,\Delta_+(\omega_2 + i\epsilon)}{[\Delta_+(\omega_1 + \omega_2 + i\epsilon)]^2}. \tag{24}$$

Incidentally, R_-, as given in Eq. (23), satisfies Eq. (21), so that the six-point amplitude obtained by continuation in g is verified to satisfy the dynamical equation with the bound-state term added.

The last amplitude, K, is to be obtained from unitarity, since K does not appear in any of the dynamical equations used for T_+, P_-, or R_-. Of course, K appears in dispersion relations obtained by contracting other variables than those contracted in obtaining Eqs. (16) and (21). However, we must be careful to see that K is consistent with the approximations we have made. In particular, we must avoid a definition of K based on dispersion relations which are not satisfied by our approximations to P_- and R_-. Since, in any event, we want a unitary scattering matrix, we use unitarity to define K. The requirement of unitarity for H is

$$\mathrm{Im}\, H(\omega) = [ku^2(\omega)/4\pi]T_-(\omega)H^*(\omega) + [\bar{k}u^2(\bar{\omega})/4\pi]H(\omega)K^*(\bar{\omega})$$
$$+ \frac{1}{16\pi^3}\int_\mu^{\omega-\mu} d\omega_1\, k_1k_{-1}u^2(\omega_1)u^2(\omega_{-1})P_-(\omega_1, \omega_{-1})J^*(\omega_1, \omega_{-1}), \tag{25}$$

where $\bar{\omega} = \omega - \omega_B$, $\omega_{-1} = \omega - \omega_1$, and $\omega > 2\mu$. Every term in Eq. (25) has been determined except K. Thus we find the equation

$$K(\omega) = M_-(\omega) + \left[\frac{g(\omega_B - \mu)\,\Delta_-(\omega + i\epsilon)\,\Delta_+(\omega_B)}{g_B(\omega + \omega_B - \mu)\,\Delta_+(\omega + \omega_B + i\epsilon)}\right]^2 [T_-(\omega + \omega_B) - M_+(\omega + \omega_B)]. \tag{26}$$

We now have all the amplitudes required to verify that the scattering matrix is unitary. In the π^+p channel, the states we retain are π^+p and $\pi^+\pi^+n$. Unitarity then relates the imaginary parts of T_+, P_+, and R_+ to quadratic forms in these amplitudes, just as it does when no bound states are present. We do not present the calculations, but simply state that the unitarity equations are satisfied. In the π^-p channel, we retain the states π^-p, π^+B^-, and $\pi^+\pi^-n$. Here, unitarity specifies the imaginary parts of T_-, P_-, R_-, H, J, and K. These equations are also satisfied.

VI. SINGULARITIES OF THE AMPLITUDE FOR $\pi^+ + B^- \to \pi^+ + B^-$

In conclusion, we examine the singularities of one of the amplitudes for scattering from the bound state. We choose the elastic scattering amplitude

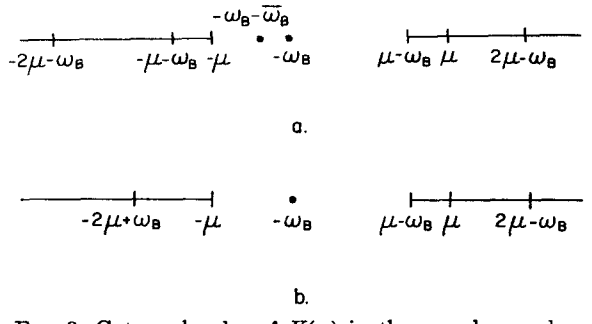


FIG. 3. Cuts and poles of $K(\omega)$ in the complex ω plane: (a) as given by Eq. (26); (b) as given by Eq. (28).

$K(\omega)$ for this purpose. Since $K(\omega)$ is unitary, its right-hand cut has the branch points corresponding to the $\pi^- p$, $\pi^+ B^-$, and $\pi^+\pi^- n$ thresholds, and the discontinuities across the cut that are specified by unitarity. The unphysical singularities we find from Eq. (26) are a pole at $\omega = -\omega_B$ with residue $-g_B^2$, a pole at $\omega = -\omega_B - \bar{\omega}_B$ with residue τ,

$$\tau = \left[\frac{G_B g(\mu - \omega_B)\,\Delta_+(\omega_B)\,\Delta_-(-\omega_B - \bar{\omega}_B)}{g_B(\mu + \bar{\omega}_B)\,\Delta_+(-\bar{\omega}_B)}\right]^2, \quad (27)$$

and branch cuts start at $-\mu$, $-\mu - \omega_B$, and $-2\mu - \omega_B$ and extending to $-\infty$. On the other hand, the correct unphysical singularities can be found from the dispersion relation for $K(\omega)$

$$K(\omega) = \sum_S \left[\frac{\langle B^-|\, j(0)\,|S\rangle\langle S|\, j^\dagger(0)\,|B^-\rangle}{E_S - m_B - \omega - i\epsilon} + \frac{\langle B^-|\, j^\dagger(0)\,|S\rangle\langle S|\, j(0)\,|B^-\rangle}{E_S - m_B + \omega + i\epsilon}\right]. \quad (28)$$

Consistent with our approximations, we retain states $n, \pi^- p, \pi^+ B^-$, and $\pi^+\pi^- n$ in the first term, and obtain the right-hand cut dictated by unitarity plus the pole at $\omega = -\omega_B$ with residue $-g_B^2$. We retain states $\pi^- B^-$ and $\pi^-\pi^- n$ in the second term, and obtain left-hand cuts beginning at $-\mu$ and $-2\mu + \omega_B$. Thus, one of the poles and two of the left-hand cuts of our approximation to $K(\omega)$ are spurious, and the crossed three-particle cut is missing. The cuts and poles of $K(\omega)$ as given by our approximation, Eq. (26), and by the dispersion relation, Eq. (28), are compared in Fig. 3. On the positive side, the direct n pole, which is the unphysical singularity nearest the physical region, is correctly given by our approximation to $K(\omega)$.

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Common Interpretation of Phase Transitions in Various Models*

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A discussion is presented of the formal analogy which exists between the Bardeen–Cooper–Schrieffer (BCS) model for superconductivity and the several variations of the model suggested by Kac for the exact study of phase transitions. Some of the algebraic techniques, pioneered by Haag for his formulation of axiomatic field theory and his application of this theory to the BCS model, are shown to extend to all these cases. Some arguments are given in the beginning of the paper to point out the necessity of a new interpretation of the existence of various phases in the same physical system. The results obtained so far for equilibrium situations confirm the consistency of the proposed tentative description of the phenomena considered.

I. INTRODUCTION

WE want to reconsider in this paper what might be the origin of the existence of sharply defined, different phases for a same, unique, and given system. As is well known, these phases have very different physical properties from one another. In particular, since the Hamiltonian of the system under consideration is supposedly known, explicitly given, and simple enough to allow exact calculations, one could even ask the question of how it is possible that the energy spectrum (i.e., not only the population of the different energy levels, but also the levels themselves) is so different in one phase from what it is in another. The case of superconductivity is a good prototype to help in crystallizing this question, and, with proper references, we shall come back to it later in this section. It seems indeed possible to associate the various phases with some characteristic excitations which diagonalize the Hamiltonian in ways which differ completely from one phase to the other. The diagonalization of a Hermitian operator is, however, a procedure which is known to give a unique solution, so that it becomes somewhat difficult to understand this aspect of the problem within ordinary (quantum) statistical mechanics, *unless* one is willing to think of these different diagonalizations as approximations. It is true that there are many physical systems (particularly in solid state physics) where, since the Hamiltonian is a complicated sum of various terms, it is both difficult and useless to try for an exact solution of the diagonalization problem. The reason for a less strict approach in these latter cases is because, in a certain range of temperature, say, certain excitations are preponderant, whereas, in a different range other excitations are preponderant. Using this reasoning, one gets different domains of validity for different approximations. However, these various domains are *not* sharply defined, rather, they are linked by some intermediary smooth transition region where neither approximation is good. This is not so for the case of superconductivity where approximation (besides the thermodynamical limit which is anyway the same for both regions involved) need not be made as soon as one agrees on an appropriate form for the interaction between Cooper pairs, and where the normal and the superconductive phases, although adjacent to each other, are sharply distinct.

To account for the sharp character of phase transition as reflected in the sharp transition from one (exact) "diagonalization" of the Hamiltonian to another, we have been led to argue in favor of the tentative interpretation that discontinuities in the equation of state are attributed to the passage from one family of Hilbert space representations of the theory to another. In conformity with the general ideas developed by Haag in his formulation of (relativistic) axiomatic field theory, there are two ingredients in any physical problem. The first is provided by the observables of the theory (or the underlying fields). To these observables one associates an algebraic structure (such as a B^*-algebra) *a priori* independent of any particular Hilbert space realization. The second ingredient is provided by the states on the system, or more precisely by an adequatedly chosen family of states. This latter choice is essentially dictated by the preparation of the system, as specified by some external parameters such as, for a spin system, the external magnetic field and the temperature. Mathematically, one associates to each state a linear func-

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tional on the algebra generated by the observables.

For an illuminatingly simple description of this approach, see for instance Haag's own lecture notes.[1]

With these two ingredients—a B*-algebra and some set of linear functionals on it—one can construct a Hilbert space representation of these two objects, respectively, as a C^*-algebra of operators and its associated density matrices (or possibly a generalization of this concept to more general functionals[2]). The representations so obtained are not necessarily equivalent, a fact which is well known in the case of the canonical commutation (or anticommutation) rules.[3] The operators corresponding to the same element of the original algebra might have quite different properties when belonging to inequivalent representations. In particular, their spectrum in general is representation-dependant.

The point now is to examine whether this approach might be of some relevance to the description of phase transitions. The core of the argument is that, for some systems known to exhibit phase transitions, different phases are associated with different sets of classes of inequivalent representations. This fact manifests itself physically by the existence of different types of excitations which exactly diagonalize the Hamiltonian, in the appropriate representation, the thermodynamical limit being taken first.

To test this interpretation, we intend to discuss in this paper some of the models, which are known to exhibit phase transitions, yet can be solved exactly, and, which, moreover, are known to have at least something in common, even if at this point this analogy appears somewhat superficial. We formulate precisely some conditions on these models in order to be able to move the analogy to a level where we can support the previously stated point of view. It appears in the course of the developments that our results present a definite formal analogy with those obtained by a brute use of the recipe known as the molecular field method (see for instance Ref. 4). However, it should be realized that the latter is, in general, to be considered only as an approximation, even if it turns out to be a very gross one. The presently proposed method differs in two aspects from the molecular field method. First, some of the necessary conditions for the validity of the present method are carefully spelled out; this is due to a difference in the mathematical techniques involved. Second, the physical interpretation of the results reflect quite a different underlying "philosophy," as we have tried to make clear in this preliminary discussion.

A good portion of this paper develops an analogy. To present this analogy naturally, we first want to recall an aspect of the Bardeen–Cooper–Schrieffer (BCS) model,[5] discovered by Haag,[6] and rediscussed later on by other authors.[7,8] Because we now know that every step of Haag's argument can be made rigorous, even in the severe standards of axiomatic field theory, we are therefore free to use a more heuristic language in the present paper, which intends to reach a wider audieace than the inner circle to whom Refs. 7 and 8 were directed.

The BCS model is described by the Hamiltonian

$$H = H_0 + \hat{H}_1 \tag{1}$$

with

$$H_0 \equiv \sum_{p,\alpha} \epsilon(p) a_\alpha^*(p) a_\alpha(p), \tag{2}$$

$$\hat{H}_1 \equiv \sum_{p,q} b^*(p) \hat{v}(p, q) b(q), \tag{3}$$

where $a_\alpha^*(p)$ and $a_\alpha(p)$ are, respectively, the creation and the annihilation operators of the unperturbed fermion excitations (electrons), with α and p denoting respectively the spin and the momentum. $b^*(p)$ is the creation operator of the Cooper pair $a_\uparrow^*(p)$, $a_-(-p)$. The "hats" recall the volume dependance of the interaction coupling constant $\hat{v}(p, q)$. The interaction $\hat{H}_1$ can be rewritten as

$$\hat{H}_1 = \sum_p b^*(p)\, \hat{\Delta}(p) \tag{4}$$

with

$$\hat{\Delta}(p) = \sum_q \hat{v}(p, q) b(q). \tag{5}$$

The volume-dependant operator (5) plays a central role in the theory. Haag's discovery was, in this connection, to see that, *if* the limit $\Delta(p)$ of $\hat{\Delta}(p)$ exists as the volume V extends to infinity, *then* this limiting operator commutes with all the field operators *provided* the condition

$$\lim_{V\to\infty} |\hat{v}(p, q)| = 0 \tag{6}$$

is satisfied; this is the case in the BCS model.

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[8] G. Emch and M. Guenin, J. Math. Phys. **7**, 915 (1966).

Now, the fact that $\Delta(p)$ belongs to the *center* of the algebra generated by the field operators is sufficient to ensure (in the infinite-volume limit) the diagonalizability of the Hamiltonian in term of quasi-particle excitations

$$H_{\text{eff}} = \sum_{p,\alpha} E(p)\gamma^*_\alpha(p)\gamma_\alpha(p) \tag{7}$$

with

$$E(p)^2 = \epsilon(p)^2 + \Delta^*(p)\,\Delta(p). \tag{8}$$

This diagonalization is obtained via a *generalized*[8] Bogoliubov–Valatin transformation, and the quasi-particle creation and annihilation operators are "linear" combinations of the particle creation and annihilation operators. The coefficients of these linear combinations depend on the energy gap. This allows the derivation of a *temperature-dependent* equation for the energy gap.[5] The solution of this equation presents a discontinuity for a certain temperature T_c above which the energy gap identically vanishes.

The system is hence characterized, for $T < T_c$, by an *effective* Hamiltonian, diagonalized in term of *temperature-dependent* quasi-particles excitations.[5] These are such that the effective Hamiltonian exhibits a nonanalytic dependance of the temperature at T_c. All of that, naturally enough, leads to a phase transition.

There is now a rather obvious question to ask, namely, whether these features (as summarized in the very last paragraph above) are strictly characteristic of superconductive metals, or whether there exists in nature (or at least in the more restricted realm of theoretical physics) some systems for which the phase transition can be described in a similar way.

The aim of the present paper is to point out that a similar treatment can be given for another model, also exactly solvable in a certain limit in which it exhibits a phase transition. This model was proposed by Kac[9] and was analyzed in detail in a whole series of subsequent papers.[10] For simplicity, we consider here its Ising model version,[11] one of its variations,[12] and a generalization of it.

This model is characterized by the following Hamiltonian:

$$H = H_0 + \hat{H}_1, \tag{9}$$

with

$$H_0 \equiv -B \sum_i \sigma^z_i, \tag{10}$$

$$\hat{H}_1 \equiv \sum_{ij'} \hat{\epsilon}_{ij'}\sigma^z_i\sigma^z_{j'}. \tag{11}$$

This Hamiltonian describes an assembly of $\frac{1}{2}$-spins ($\mathbf{s}_i = \frac{1}{2}\boldsymbol{\sigma}_i$) placed at fixed lattice sites (originally a one-dimensional chain) and submitted to an homogeneous magnetic field **B**. The spin–spin interaction coupling $\hat{\epsilon}_{ij'}$ depends on a parameter γ, and on the distance $||j - j'||$ between the sites j and j', in the following way

$$\hat{\epsilon}_{ij'} = -(1 - \delta_{ij'})\alpha\gamma \exp(-\gamma\,||j - j'||). \tag{12}$$

A phase transition is known to arise when the lattice is infinite *and* the limit of γ going to zero is taken (for the "thermodynamical" and "van der Waals" limits, respectively).

The analogy between Eqs. (1)–(3) and (9)–(11) is appealing if one notices, moreover, that in both models the effect of the limiting procedure is to make the coupling constant go to zero.

This feeling is still strengthened if one remembers that Mermin's model also exhibits the same features. The Hamiltonian of this last model is[12]

$$H = H_0 + \hat{H}_1 \tag{13}$$

with

$$H_0 = -B \sum_{i=1}^{N} \sigma^z_i + B \sum_{i=N+1}^{2N} \sigma^z_i, \tag{14}$$

$$\hat{H}_1 = -\alpha \cdot \frac{1}{2N} \sum_{ij'} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{j'}. \tag{15}$$

In this model again a phase transition occurs in the limit of infinite N. Our analogy is hence deeper than just the superficial analogy which exists between the *field operators* appearing in the interaction Hamiltonian.[13] It really has to do with the *spacial dependance* (either in momentum or in configuration space) *of the interaction coupling constant.*

II. SOLUTION OF THE $\frac{1}{2}$-SPIN MODELS.

Consider an assembly of $\frac{1}{2}$-spins placed at the fixed sites $\{j\}$ of an arbitrary lattice and submitted to an inhomogeneous magnetic field, the direction of which, however, is kept fixed for simplicity. The Hamiltonian of this system is then

$$H = H_0 + \hat{H}_1, \tag{16}$$

[9] M. Kac, Phys. Fluids **2**, 8 (1959).

[10] M. Kac, G. E. Uhlenbeck, and P. C. Hemmer, J. Math. Phys. **4**, 216 (1963); G. E. Uhlenbeck, P. C. Hemmer, and M. Kac, *ibid.* 229 (1963); P. C. Hemmer, M. Kac, and G. E. Uhlenbeck, *ibid.* **5**, 60 (1964); P. C. Hemmer, *ibid.* **5**, 75 (1964).

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[12] N. D. Mermin, Phys. Rev. **A134**, 112 (1964).

[13] P. W. Anderson, Phys. Rev. **112**, 1900 (1958).

with

$$H_0 \equiv -\sum_i B_i \sigma_i^z, \tag{17}$$

$$\hat{H}_1 \equiv -\sum_{ii'} \{\hat{\epsilon}_{ii'}\sigma_i^z\sigma_{i'}^z + \hat{\eta}_{ii'}(\sigma_i^x\sigma_{i'}^x + \sigma_i^y\sigma_{i'}^y)\}, \tag{18}$$

and

$$\begin{aligned} &\hat{\epsilon}_{ii'}\ \delta_{ii'} = 0 = \hat{\eta}_{ii'}\ \delta_{ii'}, \\ &\hat{\epsilon}_{ii'} = \hat{\epsilon}_{i'i} = \hat{\epsilon}_{ii'}^*, \qquad \hat{\eta}_{ii'} = \hat{\eta}_{i'i} = \hat{\eta}_{ii'}^*. \end{aligned} \tag{19}$$

We only suppose for the moment that the coupling constants $\hat{\epsilon}_{ii'}$ and $\hat{\eta}_{ii'}$ depend on a parameter γ in a way such that

$$\begin{aligned} &\lim_{\gamma\to 0} \hat{\epsilon}_{ii'}(\gamma) = 0, \\ &\lim_{\gamma\to 0} \hat{\eta}_{ii'}(\gamma) = 0. \end{aligned} \tag{20}$$

Clearly enough, all the spin models discussed in the introduction are contained as particular cases in the present model. Further conditions, besides (16) and (17) can also be introduced later to ensure the existence of the various limits yet to be considered.

To carry out the analysis at a minimum cost, it is convenient (but not necessary) to introduce the creation and annihilation *fermion* operators $a_\alpha^*(j)$ and $a_\alpha(j)$ with α running over the two spin orientations $+$ and $-$, satisfying the canonical anticommutation rules

$$\begin{aligned} &[a_\alpha(j), a_\beta^*(j')]_+ = \delta_{\alpha\beta}\ \delta_{jj'}, \\ &[a_\alpha(j), a_\beta(j')]_+ = 0. \end{aligned} \tag{21}$$

Let us now introduce in (17) and (18) the substitution

$$\begin{aligned} &\sigma^z \to (a_+^* a_+ - a_-^* a_-), \\ &\sigma^+ \to a_+^* a_-. \end{aligned} \tag{22}$$

With this substitution in mind, let us now determine the proper quasiparticle excitations, following the method used for the BCS model.

We have [remembering conditions (19)]

$$\begin{aligned} [H, a_\pm^*(j)] &= -\hat{B}_j a_\pm^*(j) - \hat{A}_j^+ a_\pm^*(j), \\ [H, a_\mp^*(j)] &= +\hat{B}_j a_\mp^*(j) - \hat{A}_j^- a_\pm^*(j), \end{aligned} \tag{23}$$

with

$$\hat{B}_j = (B_j + \hat{A}_j^z) \tag{24}$$

and

$$\hat{A}_j^\alpha = 2\sum_{j'} \hat{\epsilon}_{jj'}^\alpha \sigma_{j'}^\alpha \qquad (\alpha = z; +; -), \tag{25}$$

where

$$\hat{\epsilon}_{jj'}^\alpha = \begin{cases} +\hat{\epsilon}_{jj'}, & (\alpha = z), \\ +2\hat{\eta}_{jj'}, & (\alpha = + \text{ or } -). \end{cases} \tag{26}$$

Now, because of (20), we have *in the limit where* $\gamma \to 0$

$$[\hat{A}_j^\alpha, a_\beta^{(*)}(j')] = 0. \tag{27}$$

[Compare to the Haag's remark stated after Eq. (5) in the Introduction.] We now suppose that

$$A_j^\alpha \equiv \lim_{\gamma\to 0} \hat{A}_j^\alpha \tag{28}$$

exists (notice that in Mermin's model, for instance, this quantity is proportional to the average of the corresponding σ^α taken over the lattice!). Then in the limit where $\gamma \to 0$, instead of (23),

$$\begin{aligned} [H, a_\pm^*(j)] &= -(B_j + A_j^z)a_\pm^*(j) - A_j^+ a_\pm^*(j), \\ [H, a_\mp^*(j)] &= +(B_j + A_j^z)a_\mp^*(j) - A_j^- a_\pm^*(j), \end{aligned} \tag{29}$$

and similarly,

$$\begin{aligned} [H, a_+(j)] &= +(B_j + A_j^z)a_+(j) + A_j^- a_-(j), \\ [H, a_-(j)] &= -(B_j + A_j^z)a_-(j) + A_j^+ a_+(j), \end{aligned} \tag{30}$$

where all the coefficients of the field operators in (29) and (30) belong to the center of the algebra generated by the field operators

$$\{a_\alpha^*(j), a_\alpha(j),\ \forall\alpha,\ \forall j\}.$$

We can now use the procedure known as the *generalized* Bogoliubov transformation[8] to find the quasiparticle excitations as solutions of the equations

$$\begin{aligned} [H, \gamma_\pm^*(j)] &= \mp B_j' \gamma_\pm^*(j), \\ [H, \gamma_\pm(j)] &= \pm B_j' \gamma_\pm(j), \end{aligned} \tag{31}$$

with

$$\begin{aligned} \gamma_+^*(j) &= u(j)a_+^*(j) + v(j)a_-^*(j), \\ \gamma_-^*(j) &= u(j)a_-^*(j) - v(j)a_+^*(j), \end{aligned} \tag{32}$$

and

$u(j)$, $v(j)$ Hermitian (see Ref. 14 below).

We moreover impose $\gamma_\pm^{(*)}$ to satisfy the canonical anticommutation rules

$$\begin{cases} [\gamma_\alpha(j), \gamma_\beta^*(j')]_+ = \delta_{\alpha\beta}\ \delta_{jj'}, \\ [\gamma_\alpha(j), \gamma_\beta(j')]_+ = 0. \end{cases} \tag{33}$$

[14] The connection with the apparent "symmetry breaking" in phase-transition phenomena, [which appears also in our treatment, as the arbitrary choice of u and v Hermitian in our Eqs. (32)] is discussed from an intuitive physical point of view in Ref. 4. Some interesting comments are also to be found in P. W. Anderson, in *Lectures on the Many-Body Problem*, E. R. Caianello, Ed. (Academic Press Inc., N. Y. 1964), Vol. 2, p. 113; and in P. W. Anderson, Rev. Mod. Phys. **38**, 298 (1966). It was mainly to this aspect of the problem in superconductivity that our Ref. 8 was devoted.

We find

$$(B_i')^2 = (B_i + A_i^z)^2 + A_i^+ A_i^-, \tag{34}$$

$$\begin{cases} u(j)^2 = \frac{1}{2}\left(1 + \frac{[B_i + A_i^z]}{B_i'}\right) \\ v(j)^2 = \frac{1}{2}\left(1 - \frac{[B_i + A_i^z]}{B_i'}\right) \end{cases} \tag{35}$$

so that the Hamiltonian can be reduced to the form

$$H_{eff} = -\sum_i B_i'[\gamma_+^*(j)\gamma_+(j) - \gamma_-^*(j)\gamma_-(j)], \tag{36}$$

i.e., with the substitution

$$\tau_i^z \leftarrow [\gamma_+^*(j)\gamma_+(j) - \gamma_-^*(j)\gamma_-(j)], \tag{37}$$

$$H = -\sum_i B_i'\tau_i^z, \tag{38}$$

the physical interpretation of which is obvious: The diagonalization procedure, as described above, leads to an "effective Hamiltonian" describing an assembly of independent "½-spins" [see Eqs. (42) and (43) below] placed at the lattice sites and now submitted to a "local magnetic field" B_i'.[15] We still have to calculate these B_i'. We again proceed as for the BCS case.[8] Let $\rho(\beta)$ be the "density matrix" describing the system at equilibrium with a thermal bath at temperature $T = (k\beta)^{-1}$. We have

$$\langle A_i^\alpha \rangle_\beta = 2 \sum_{i'} \epsilon_{ii'}^\alpha \langle \sigma_{i'}^\alpha \rangle_\beta. \tag{39}$$

We then express σ_i^α and $\rho(\beta)$ in term of quasi-particle excitations and take the limit for $\gamma \to 0$ to get

$$A_{i'}^{\parallel}(\beta) \equiv \langle A_{i'}^z \rangle_\beta = \lim_{\gamma \to 0} 2 \sum_i \hat{\epsilon}_{ii'} \frac{[B_i + A_i^{\parallel}(\beta)]}{B_i'(\beta)} \tanh\{\beta B_i'(\beta)\}, \tag{40}$$

$$A_{i'}^{\perp}(\beta) \equiv \langle A_{i'}^+ \rangle_\beta = \langle A_{i'}^- \rangle_\beta = \lim_{\gamma \to 0} 2 \sum_i \hat{\eta}_{ii'} \frac{A_i^{\perp}(\beta)}{B_i'(\beta)} \tanh\{\beta B_i'(\beta)\}. \tag{41}$$

Equations (40) and (41) show an expected formal similarity with the BCS gap equation. Their interpretation, however, differs from case to case. They were obtained through a rather straightforward calculation. In this connection, we only want to mention that we used the following substitutions, suggested by (22), (37), and (32):

$$\begin{aligned} \sigma_i^z &\leftrightarrow (u_i^2 - v_i^2)\tau_i^z - 2u_i v_i(\tau_i^+ + \tau_i^-), \\ \sigma_i^+ &\leftrightarrow u_i v_i \tau_i^z + u_i^2 \tau_i^+ - v_i^2 \tau_i^-, \\ \sigma_i^- &\leftrightarrow u_i v_i \tau_i^z + u_i^2 \tau_i^- - v_i^2 \tau_i^+, \end{aligned} \tag{42}$$

and

$$\begin{aligned} \tau_i^+ &\leftrightarrow \gamma_+^*(j)\gamma_-(j), \\ \tau_i^- &\leftrightarrow \gamma_-^*(j)\gamma_+(j). \end{aligned} \tag{43}$$

The very existence of the transformations (42) (where the quasi-spin operators are expressed as "linear" combinations[15] of the original spin operators) suggests that the whole analysis, as carried out in the section, could be done without introducing the fermion field operators at all. *This is indeed the case.* However, we kept the presently given derivation to emphasize the complete (but formal) analogy between the BCS model and the models considered here. One main difference, especially from the physical point of view, is that the present interaction suggests working in the configuration space, whereas the BCS interaction is appropriately treated in the momentum space. The methods are hence only formally identical, whereas the physical content of the two theories is somewhat different, as is to be expected! This enhances the interest of the present unifying analogy.

III. THE WEISS MODEL

The most elementary application of the analysis carried out above is the so-called Weiss model, where

$$B_i = B, \qquad \forall_i, \tag{44}$$

$$\hat{\epsilon}_{ii'} = g/2N, \qquad \forall_{i,i'}, \tag{45}$$

$$\hat{\eta}_{ii'} = 0, \qquad \forall_{i,i'}, \tag{46}$$

(N is the number of spin sites). We have in this case

$$\langle A^{\perp} \rangle_\beta = 0, \tag{47}$$

$$B'(\beta) = B + \langle A^{\parallel} \rangle_\beta, \tag{48}$$

$$\tau_i^z \leftrightarrow \sigma_i^z, \tag{49}$$

and consequently

$$H(\beta) = -\sum_i (B + \langle A^{\parallel} \rangle_\beta)\sigma_i^z \tag{50}$$

and

$$\langle \sigma_i^z \rangle_\beta = \tanh\{\beta(B + \langle A^{\parallel} \rangle_\beta)\}, \tag{51}$$

[15] Here again there exists a definite semantic analogy with the molecular field method. One should however realize that the A_i^α are *not* scalars, but are more general operators belonging to the *center* of the algebra generated by the field operators. In this connection, we also have to recall that the use of inequivalent (irreducible) representations of the *same* algebra, as suggested by Refs. 6–8, is dictated by the different canonical equilibrium linear functionals $< >_\beta$. It reflects then in the spectrum of the Hamiltonian. This is in conformity with the general idea that, whereas the algebra of the field operators is a fixed object for the theory, the choice among its various representations depends ultimately on the use one wants to make of them (in particular, this choice might be suggested, as is done here, by the preparation of the system, as expressed by B and β).

where $\langle A^{\|} \rangle_{\beta}$ is determined by (40) which in this case reduces to:

$$\langle A^{\|} \rangle_{\beta} = g \tanh \{\beta(B + \langle A^{\|} \rangle_{\beta})\}. \qquad (52)$$

Equations (51) and (52) correspond indeed to the result obtained directly by the Weiss molecular field method. Hence, reduced to this case, our analysis simply consists in *proving* that the molecular field method is justified in the infinite "volume" limit, a result which was already admitted for a long time on the ground of more or less heuristic arguments.

The characteristic features of the Weiss model are well known, and the discussion is indeed straightforward as soon as one gets Eqs. (51) and (52). Let us therefore only recall that the phase transition obtained in the Weiss model is the magnetic analog of the phase transition described by the van der Waals equation. It is therefore not too surprising that the models of Kac and co-workers also lead to such an equation, since they also satisfy the assumptions under which our derivation is valid. There is obviously more than just that in Refs. 9 to 11. A detailed discussion of some of the other aspects of the Kac models is presented in another publication.[16]

IV. CONCLUSIONS

Our treatment is manifestly much more general than the Weiss model considered in Sec. III above. Besides the various models satisfying directly the assumptions under which the derivation given in Sec. II apply without any change, there indeed exist several other models also amenable to a similar form by an appropriate "canonical" transformation. However, for the sake of keeping this paper within reasonable length, we postpone the treatment of more sophisticated models to the following paper.[16] For the time being, we want to point out an analogy which, although formal, might turn out to be a useful one. It indicates that a description of at least a wide class of phase-transition models might be given in the following terms.

First of all, as in all other treatments, a limiting procedure (in which the volume of the system, as well as related quantities, go to infinity) has to be taken. This is nothing other than the usual "thermodynamical limit", completed by appropriate conditions on the spacial dependence of the interaction coupling constant.

Then, in this limit, the Hamiltonian can be diagonalized into an "effective Hamiltonian" expressed in term of *temperature-dependent* "quasi-particle excitations" (defined in different Hilbert spaces!).

The temperature dependence of both equilibrium and nonequilibrium properties can then be traced directly to this effective Hamiltonian, respectively through the partition function and the time-evolution operator.[17]

The views presented in this paper might then turn out to open the way to a unified interpretation of the occurence of singularities in both equilibrium and nonequilibrium properties. These, however, have to be discussed from case to case for a more detailed information.[16] Hopefully, it becomes easier to obtain when the present scheme is used.

Finally, we want to stress that the effort to comprehend the existence of phase transitions in several systems as the occurence of quasi-particle excitations is not new.[4,14] We only claim to have outlined a consistent approach with a mathematically meaningful description of the actual procedure involved.

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[16] G. Emch, J. Math. Phys. **8**, 19 (1967), where the equilibrium properties, and, in particular, the equation of state, are discussed as particular cases of the theory given in the present paper.

[17] Although the latter might present specific problems which we intend to come back in a forthcoming publication.

van der Waals Wiggles, Maxwell Rule, and Temperature-Dependent Excitations*

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Starting from a temperature-independent Hamiltonian, we discuss for some models the coexistence of the van der Waals wiggles and the Maxwell–van der Waals isotherms. The main tool of this paper is provided by the temperature-dependent excitations techniques developed in an earlier paper. Some ferromagnetic models and lattice-gas models are treated along similar lines. The van der Waals wiggles and the Maxwell–van der Waals isotherms appear below the critical temperature as two solutions of a system of self-consistent equations. The choice between the two solutions is then dictated by energy considerations.

I. INTRODUCTION

THE "correct" equations of state for a liquid–vapor system at thermal equilibrium below the critical temperature are usually obtained from the van der Waals theory by a trick, known as the Maxwell equal-area construction. This construction predicts the position of the plateau in the pressure–density diagram. However, it suffers from two defects. First, the "physical arguments" on which it is based have more to do with the thermodynamics of the macroscopic description than with the mechanism of the microscopic description. In that sense, this construction, as such, is not fully satisfying from the point of view of statistical mechanics. Second, as soon as one is willing to accept the Maxwell construction, one has troubles trying to invalidate it in order to allow the understanding of the existence of the supercooling and superheating phenomena as "excited meta-stable situations." Similar problems occur in the study of magnetic systems.

There is hope that some simple models, in spite of their admitted crudeness, might give some insight into this old puzzle. The models proposed by Kac and co-workers[1] are certainly among the most interesting and the most successful attempts for a justification of the Maxwell–van der Waals isotherms. It is, however, difficult to convince oneself that the techniques used by these authors really belong to the problem at hand. It is also not quite clear, whether the supercooling and the superheating phenomena can find a place in that type of discussion.

In this paper, we keep the main idea underlying the investigations of Ref. 1, namely, that the liquid–vapor system is properly described through a two-body potential with an infinitely repulsive hard core followed by an "infinitely weak," "infinitely long-range," attractive part. For the sake of simplicity, we, however, first consider an even more schematic potential than that proposed by Kac and co-workers. This choice was deliberately made on the grounds of the resulting conciseness; we know[2] that more general potentials, including that of Kac, can be treated by techniques similar to those to be used hereafter. (Some conditions imposed in the first sections are, in particular, released in Sec. V, as to include, among many other cases, the Kac potential.) We would like to suggest that the present techniques are more genuinely proper to the physics of systems exhibiting phase transitions, even if one might object to the oversimplifications attached to the workable models.

II. MAGNETIC CASE

We first want to discuss the case of a lattice of N sites, placed in a magnetic field B, with a spin-$\frac{1}{2}$ particle sitting on each site of it. We assume that the Hamiltonian of this system is of the form

$$H = H_0 + V \tag{1}$$

with

$$H_0 = -B \sum_i \sigma_i^z, \tag{2}$$

$$V = -\frac{\alpha^{\parallel}}{2N} \sum_{ii'} \sigma_i^z \sigma_{i'}^z - \frac{\alpha^{\perp}}{2N} \sum_{ii'} (\sigma_i^x \sigma_{i'}^x + \sigma_i^y \sigma_{i'}^y). \tag{3}$$

This is a particular case of the general case treated in Sec. II of Ref. 2, and the Heisenberg generaliza-

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[1] M. Kac, Phys. Fluids 2, 8 (1959). M. Kac, G. E. Uhlenbeck, and P. C. Hemmer, J. Math. Phys. 4, 216 (1963); G. E. Uhlenbeck, P. C. Hemmer, and M. Kac, *ibid.* 4, 229 (1963); P. C. Hemmer, M. Kac, and G. E. Uhlenbeck, *ibid.* 5, 60 (1964); P. C. Hemmer, *ibid.* 5, 75 (1964); M. Kac and E. Helfand, *ibid.* 4, 1078 (1963); E. Helfand, *ibid.* 5, 127 (1964).

[2] G. Emch, J. Math. Phys. 8, 13 (1967).

tion of the particular example given in Sec. III of this same paper. (Here again, the dimensionality of the lattice is not relevant for our considerations.) We know from this earlier publication that the Hamiltonian (1) can be "diagonalized," for $N \to \infty$ (and any reciprocal temperature β) as

$$H_{\text{eff}}(\beta) = -B'(\beta) \sum_i \tau_i^z(\beta) \tag{4}$$

with

$$B'(\beta)^2 = [B + A^{\parallel}(\beta)]^2 + A^{\perp}(\beta)^2, \tag{5}$$

$$A^{\parallel}(\beta) = \alpha^{\parallel}\{[B + A^{\parallel}(\beta)]/B'(\beta)\} \tanh [\beta B'(\beta)], \tag{6}$$

$$A^{\perp}(\beta) = \alpha^{\perp}[A^{\perp}(\beta)/B'(\beta)] \tanh [\beta B'(\beta)]; \tag{7}$$

$$\tau_i^z(\beta) = [u(\beta)^2 - v(\beta)^2]\sigma_i^z - 2u(\beta)v(\beta)(\sigma_i^+ + \sigma_i^-), \tag{8}$$

$$\begin{aligned} u(\beta)^2 &= \tfrac{1}{2}\{1 + [B + A^{\parallel}(\beta)]/B'(\beta)\}, \\ v(\beta)^2 &= \tfrac{1}{2}\{1 - [B + A^{\parallel}(\beta)]/B'(\beta)\}. \end{aligned} \tag{9}$$

Equations (5)–(7) form a set of coupled equations, the solutions of which we want to analyze in term of the macroscopic (M, B) diagram. The magnetization M per spin is defined as usual by

$$M \equiv \frac{1}{N}\frac{\partial}{\partial B} \ln \operatorname{Tr} e^{-\beta H}, \tag{10}$$

which reduces here to

$$M(\beta) = (\partial B'/\partial B) \tanh \beta B' = \langle \sigma^z \rangle_\beta = A^{\parallel}(\beta)/\alpha^{\parallel}. \tag{11}$$

A first solution is

$$A^{\perp}(\beta) = 0, \tag{12}$$

$$B'(\beta) = B + A^{\parallel}(\beta), \tag{13}$$

$$M(\beta) = \tanh \{\beta[B + \alpha^{\parallel}M(\beta)]\}. \tag{14}$$

We recognize in (14) the equation of state found in Ref. 2 for the Ising equivalent of our present generalized Heisenberg model. It is the normal *van der Waals solution* of the *Weiss model*. It exists for all temperatures and exhibits its famous wiggles for

$$T < T_c^{\parallel} \equiv \alpha^{\parallel}/k. \tag{15}$$

In our present model, however, a second solution might manifest itself for

$$T < T_c^{\perp} \equiv \alpha^{\perp}/k, \tag{16}$$

which we refer to as the *Maxwell solution*. It is

$$A^{\perp}(\beta) \neq 0, \tag{17}$$

$$B'(\beta) = \alpha^{\perp} \tanh [\beta B'(\beta)], \tag{18}$$

$$M = B/(\alpha^{\perp} - \alpha^{\parallel}). \tag{19}$$

Two short remarks are in order here. First, one should notice that (16) is a necessary, but not sufficient, condition for the existence of the Maxwell solution; further conditions are imposed by Eqs. (5) and (18) so that the Maxwell solution indeed disappears for too large values of B, even if (16) is satisfied. There is, however, no point in elaborating more on this fact here. Second, and more important, for the Maxwell solution (whenever it exists), M depends only on B, and not on β. Hence, the Maxwell isotherms, in the magnetic case, overlap each other.

In summary, we see that, in the neighborhood of $B = 0$, two solutions of the equations of state actually *coexist*: the van der Waals solution (14) and the Maxwell solution (19). Among the several differences in character between these two solutions, only the most essential for our discussion is emphasized here, namely the following. Along any van der Waals isotherm, the energy per spin

$$E(\beta) \equiv (1/N) \times \operatorname{Tr} \{H(\beta) \exp [-\beta H(\beta)]\}/\operatorname{Tr} \{\exp [-\beta H(\beta)]\} \tag{20}$$

varies with the value of the magnetization M. On the contrary, the energy of a state from the Maxwell solution is constant along each Maxwell isotherm and hence depends on the temperature only. This difference allows us to determine quite easily which is the fundamental state at a given temperature, and at a given magnetic field. In particular, when the anisotropy goes to zero, the isotherms for the *fundamental* states are the desired Maxwell–van der Waals isotherms. Below the critical temperature, they are continuous but only piecewise-analytic. For every temperature above the critical temperature, we have only one solution to choose from: the van der Waals isotherm which is perfectly well behaved in this region (in particular, $\partial p/\partial \rho$ is everywhere positive).

In this derivation, the Maxwell–van der Waals isotherms appear as direct consequences of the long-range Heisenberg-like interaction (3) we started from. This might be considered as quite a gratifying fact, since an Heisenberg-like model is *a priori* physically more suitable than its truncated Ising-like version for which, as we know (Ref. 2, Sec. III), the van der Waals wiggles appear without any Maxwell counterpart. (This statement is to be qualified in Sec. V.)

This derivation, moreover, seems to give some definite support to the view that the analytical prolongations of the van der Waals isotherms inside the plateau region have a physical meaning and correspond to true equilibrium states of the system,

lying, however, higher in energy than the corresponding states of the Maxwell solution. We also want to notice for completeness that no such prolongation of the Maxwell isotherms mathematically exists outside the plateau region; this agrees with the physical expectation. Finally, as in all similar cases, a weak perturbation, not included in (3), might turn into meta-stable states, the states which appear here on the equilibrium, but not fundamental, van der Waals wiggles. This aspect of the problem is, however, beyond our scope here.

III. SPINLESS FERMI LATTICE-GAS

The next question is to find the lattice-gas analog of the magnetic case discussed in the previous section. The Ising model, from which the lattice-gas was originally modeled is, in fact, known to be a problem pertaining to classical, rather than to quantum, statistical mechanics: spin-$\frac{1}{2}$ particles are introduced at the beginning, but nothing from their quantum structure is subsequently used in the standard treatments of the Ising model (see for instance Chaps. 16 and 17 of Ref. 3). This is *a fortiori* true for the usual formulation of the lattice-gas. In the discussion presented in Sec. II, the generalization of the (classical) Ising-like model to a (quantum) Heisenberg-like model was quite obvious from both the physical and the mathematical points of view. This is not so for the lattice-gas.

Our problem is now first to find the appropriate lattice-gas equivalent of the long-range model treated in Ref. 2, Sec. III. This could obviously be done through a slight generalization of the well-known translation table (see Ref. 3) between the Ising model and the ordinary lattice-gas. We proceed, however, along a path which makes easier the formulation of the lattice-gas equivalent of our Heisenberg-like model.

We do not lose too much of the usual picture of the classical lattice-gas if we describe it as a lattice with N sites, each of which can be occupied by at most one particle. Nearest-neighbor particles, when present, interact to give rise to a constant, negative contribution to the total energy of the system. One calculates from the (grand) canonical partition function, *in the limit where N goes to infinity*, the relative number of occupied sites, and related quantities to which one associates a physical meaning as thermodynamical functions. The results so obtained turn out to be in relatively good agreement with the actual features of vapor–liquid systems.

[3] K. Huang, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1963).

A seemingly natural way to treat this model is to describe the particles at the lattice sites as interacting spinless fermions. Let us hence introduce the number operators

$$n_i = a_i^* a_i, \qquad j = 1, 2, \cdots, N \tag{21}$$

and the creation and annihilation fermion operators

$$\begin{cases} [a_j, a_{j'}^*]_+ = \delta_{jj'}, \\ [a_j, a_{j'}]_+ = 0. \end{cases} \tag{22}$$

We also want to formulate the model in a way such that the interaction is no longer restricted to nearest-neighbor particles. We hence assume the "Hamiltonian" to be of the form

$$H = -\sum_j \mu_j n_j - \sum_{jj'} v_{jj'} n_j n_{j'}. \tag{23}$$

Compare with the similar starting point taken in Chap. 3, Sec. 2 of Ref. 4.

The Hermiticity of the Hamiltonian is ensured by

$$\mu_j = \mu_j^*; \quad v_{jj'} = v_{j'j}; \quad v_{jj'} = v_{jj'}^*, \quad \text{for all } j, j' \tag{24}$$

We moreover suppose that the coupling constants $v_{jj'}$ depend on a parameter γ and that we are interested in the thermodynamical limit, where γ goes to zero and

$$\lim_{\gamma \to 0} v_{jj'} = 0. \tag{25}$$

We finally assume that the $v_{jj'}$ satisfy, as γ goes to zero, all the conditions required for the existence of all the limits we are to consider below (See Refs. 2 and 5).

The same arguments as those developed in Ref. 2 lead now to the introduction of the following *temperature-dependent effective* Hamiltonian:

$$H_{\text{eff}}(\beta) = -\sum_j \mu_j'(\beta) n_j \tag{26}$$

with

$$\mu_j'(\beta) = \mu_j + A_j(\beta), \tag{27}$$

where

$$A_j(\beta) = \lim_{\gamma \to 0} 2 \sum_{j'} v_{jj'}(\gamma) \langle n_{j'} \rangle_\beta. \tag{28}$$

These three equations combine into a self-consistency condition. In the particular case where

$$\begin{cases} v_{jj'} = a/(4N); \qquad \mu_j = \mu, \qquad \text{for all } j, j', \\ \gamma = 1/N, \end{cases} \tag{29}$$

[4] R. H. Brout, *Phase Transitions* (W. A. Benjamin Company, Inc., New York, 1965).

[5] G. Emch and M. Guenin, J. Math. Phys. **7**, 915 (1966). There is no point to open here again the mathematical discussions conducted in this reference. These are in fact immediately transferable to the present paper. We indeed want to concentrate now on the physical aspect of a similar problem.

Eqs. (26), (27), and (28) lead directly to

$$\rho(\beta) = \tfrac{1}{2}(1 + \tanh\{(\beta/2)[\mu + a\rho(\beta)/2]\}), \tag{30}$$

where the *density* ρ is defined as

$$\rho(\beta) = \lim_{N\to\infty} \langle \sum_i n_i \rangle_\beta / N. \tag{31}$$

Equation (30) is well known[4] as the lattice-gas analog of the Weiss model. It appears here as the exact analog of our Eq. (14).

To collect our thoughts, let us recall that the equation so obtained leads[4] to the equation of state

$$p + a\rho^2 = -kT \ln(1 - \rho). \tag{32}$$

This equation is close enough to the original van der Waals equation

$$p + a\rho^2 = +kT\rho/(1 - \rho) \tag{33}$$

to be worth studying. In particular, it presents the van der Waals wiggles, very much like (14) itself. As to be expected, we do not have, with this lattice-gas model, any abnormal solution of the Maxwell type in the sense of Sec. II. (See, however, Sec. V.) One of the possible reasons is that we did not introduce in our lattice-gas Hamiltonian (23) any term which could play the role of the second term present in the magnetic interaction (3). This last term could most conveniently be expressed as a sum of terms of the form $\sigma_j^+\sigma_{j'}^-$. It links two operators: σ_j^+ which rises the unperturbed energy at site j, and $\sigma_{j'}^-$ which lowers it at site j'. To pursue the analogy sketched in the beginning of this section, one might be tempted to argue that the proper generalization of (23) is to add to it a term of the form

$$V = -\sum_{ij'} w_{ij'} a_i^* a_{j'}. \tag{34}$$

However, contrary to the second term in (3), (34) is quadratic in the field operators, and can therefore, together with the unperturbed part of (23), be exactly diagonalized, even in the case of finite N, to lead to temperature-independent excitations. Consequently, even if (34) heuristically seems to be the appropriate translation of the second term of (3), it completely looses the mathematical parallelism between the two models. In particular, no Maxwell solution could appear as a result of our discussion of the equations of state. This is just another reason which prompts us to look for a more appropriate model of the lattice-gas. This is our attempt in the next section.

IV. REFINED VERSION OF THE FERMI LATTICE-GAS

Instead of allowing each site (or cell) of the lattice to be occupied by one particle at most, we now want to take cells twice the size of those considered in Sec. III. To achieve this in a convenient way, we introduce at this point two kinds of spinless fermions, visiting each of the N sites of a lattice, with the Hamiltonian

$$H_0 = \sum_{\alpha=1}^{2} H_\alpha + V_0, \tag{35}$$

where

$$H_\alpha = -\sum_j \mu_\alpha(j) n_\alpha(j) - \sum_{jj'} v_\alpha(j, j') n_\alpha(j) n_\alpha(j'), \tag{36}$$

$$V_0 = -\sum_{jj'} v_0(j, j') n_1(j) n_2(j'), \tag{37}$$

with

$$n_\alpha(j) = a_\alpha^*(j) a_\alpha(j), \quad \alpha = 1, 2; \quad j = 1, 2, \cdots, N, \tag{38}$$

and

$$\begin{cases} [a_\alpha(j), a_\beta^*(j')]_+ = \delta_{\alpha\beta}\,\delta_{jj'}, \\ [a_\alpha(j), a_\beta(j')]_+ = 0. \end{cases} \tag{39}$$

Moreover, we assume that the $v_\alpha(j, j')$ with $\alpha = 1, 2, 0$ satisfy the same conditions as the $v_{jj'}$ of Sec. III. We can hence "diagonalize" (35) in the same way as (23). In particular, if

$$\begin{cases} \mu_\alpha(j) = \mu, & \alpha = 1, 2; \quad j = 1, 2, \cdots, N, \\ v_\alpha(j, j') = a/(8N), & \alpha = 1, 2; \quad j, j' = 1, 2, \cdots, N, \\ v_0(j, j') = a/(4N), & j, j' = 1, 2, \cdots, N, \end{cases} \tag{40}$$

we get, in the limit $N \to \infty$, exactly the same equations of state as before, namely (30) or (32); now, instead of (31):

$$\begin{cases} \rho(\beta) = \tfrac{1}{2} \sum_\alpha \rho_\alpha(\beta), \\ \rho_\alpha(\beta) = \lim_{N\to\infty} \langle \sum_j n_\alpha(j) \rangle_\beta / N, \end{cases} \tag{41}$$

as was to be expected, since what we did up to now was equivalent to a relabeling of the $2N$ sites of a lattice, as suggested by the introduction of this section. However, we are now in the position to translate for this lattice-gas model the results obtained in Sec. II for our Heisenberg-like magnetic model. Let us consider the Hamiltonian

$$H = H_0 + V, \tag{42}$$

where H_0 is the Hamiltonian (35) and

$$V = -\sum_{j,j'} w_{jj'} a_1^*(j) a_2^*(j') a_2(j') a_1(j'). \tag{43}$$

We should notice at this point that this choice for the interaction makes it closer (so far as its

mathematical form is concerned) to the pair–pair interaction occurring in the Bardeen–Cooper–Schrieffer (BCS) model, than to the spin–spin interaction present in the magnetic model. However, the physical content of this model is shown to be quite similar to that of our magnetic model.

To demonstrate in a more transparent way the essence of the method, we again consider a particularly simple case, namely that prescribed by conditions (40) completed now by

$$w_{ii'} = b/(2N), \qquad j = 1, 2, \cdots, N. \tag{44}$$

From our standard diagonalization procedure,[2] we get

$$H_{\text{eff}}(\beta) = -\mu'(\beta) \sum_{\alpha,j} \gamma_\alpha^*(j)\gamma_\alpha(j) \tag{45}$$

with the temperature-dependent excitations

$$\begin{cases} \gamma_1^*(\beta) = u(\beta)a_1^*(j) + v(\beta)a_2(j), \\ \gamma_2^*(\beta) = u(\beta)a_2^*(j) - v(\beta)a_1(j), \end{cases} \tag{46}$$

where

$$\begin{cases} u(\beta)^2 = \tfrac{1}{2}[1 + (\mu + a\rho(\beta)/2)/\mu'(\beta)], \\ v(\beta)^2 = \tfrac{1}{2}[1 - (\mu + a\rho(\beta)/2)/\mu'(\beta)], \end{cases} \tag{47}$$

which are ultimately determined from the self-consistency conditions

$$\mu'(\beta) = [\mu + a\rho(\beta)/2]^2 + \nu(\beta)^2, \tag{48}$$

$$\rho(\beta) = \tfrac{1}{2}(1 + \{[\mu + a\rho(\beta)/2]/\mu'(\beta)\} \tanh [\beta\mu'(\beta)/2]), \tag{49}$$

$$\nu(\beta) = (b/4)[\nu(\beta)/\mu'(\beta)] \tanh [\beta\mu'(\beta)/2]. \tag{50}$$

A comparison of Eqs. (4)–(9), respectively, with Eqs. (45), (48), (49), (50), (46), and (47) from one side, and a comparison of Eqs. (48)–(50) with the equation of state (30), should convince the reader that we obtained here the exact lattice-gas analog of the magnetic model discussed in Sec. II. In particular, all of our discussion on the coexistence below the critical temperature of the van der Waals and the Maxwell solutions remains the same, giving rise to the famous Maxwell plateau in the pressure–density diagram.

V. COMPARISON WITH OTHER RESULTS

In Sec. II we considered, as extreme cases of a unified treatment, both the Ising and the Heisenberg magnetic couplings with a Weiss space-independent interaction. We emphasized that an exact solution of the former model can only lead to van der Waals-like isotherms, whereas the van der Waals–Maxwell isotherms appear as natural solutions of the later model, where, however, the analytic prolongations of the van der Waals isotherms into the "plateau region" still exist as excited meta-stable states. The lattice-gas analogs of these models were studied in Secs. III and IV, respectively, and shown to exhibit essentially the same features as their respective magnetic analogs, as was to be expected.

On the other hand, Kac and co-workers[1] obtained directly the van der Waals–Maxwell isotherms from a model apparently quite similar to that of Sec. III, rather than that of Sec. IV.

We therefore have two widely different methods, both claiming to be exact in the *same* limit, and apparently leading, however, to opposite conclusions. To be able to claim that our method is of some general interest, we should at least understand the difference between the results of Kac and co-workers[1] and ours.

This is indeed possible, and the aim of the present section is precisely to show how. An answer can, in fact, be found through a comparison with the arguments developed by van Kampen[6] in his version of the Kac model. Although this is hardly necessary, we make the comparison easier by taking exactly van Kampen's model which contains in some sense the Weiss-like models as particular cases. We thus apply our techniques to this model itself.

We again consider the thermodynamical and the van der Waals limits of a spinless Fermi lattice-gas with two-body interactions, as in Sec. III. We moreover introduce first van Kampen's trick and divide the lattice into M cells each containing Δ sites. The position of a site is then denoted by two indices (α, j) running, respectively, from 1 to M and from 1 to Δ. The Hamiltonian corresponding to (23) can then be rewritten as

$$H = -\mu \sum_{\alpha,j} n_\alpha(j) - \tfrac{1}{2} \sum_{\alpha,j,\alpha',j'} w_{\alpha\alpha'}(j, j')n_\alpha(j)n_{\alpha'}(j') \tag{51}$$

with

$$n_\alpha(j) = a_\alpha^*(j)a_\alpha(j) \tag{52}$$

[6] N. G. van Kampen, Phys. Rev. **A135**, 362 (1964). Several papers by S. Katsura should also be mentioned in this connection, although the methods used by this author are quite different from ours. See in particular: S. Katsura, Progr. Theoret. Phys. (Kyoto) **13**, 571 (1955), where he discusses also the Weiss model which, incidentally, he calls adequately enough the Husimi–Temperley model. There is a definite agreement between several, but not all, of Katsura's results and ours. We, however, feel that our arguments are much closer, both in their premises and their conclusions, to those of van Kampen than to those of Katsura. The latest of Katsura's papers, in which plenty of references can be found to previous works, is S. Katsura and S. Inawashiro, J. Math. Phys. **6**, 1916 (1965). In this later connection, we would like to mention that the exact model recently considered by these authors can also be treated by our method.

and

$$\begin{cases}[a_\alpha(j),\, a^*_{\alpha'}(j')]_+ = \delta_{\alpha\alpha'}\,\delta_{jj'}, \\ [a_\alpha(j),\, a_{\alpha'}(j')]_+ = 0. \end{cases} \tag{53}$$

We again assume that the potential is long-range, and to keep close to van Kampen's model, we moreover assume that the interaction between two fermions depends only on the cells in which they are

$$w_{\alpha\alpha'}(j,\, j') = w_{\alpha\alpha'}. \tag{54}$$

We suppose, as in the rest of this paper, that the w's depend on a parameter γ such that the van der Waals limit can be considered in a meaningful way (see preceding sections). At this stage, we notice that we would recover exactly the situation of Sec. III if we would also assume that [see condition (29)]

$$w_{\alpha\alpha'} = a/(2\,\Delta M). \tag{55}$$

The point is, however, not to restrict $w_{\alpha\alpha'}$ by (55), as it is discussed below.

Our Hamiltonian (51) can now be rewritten as

$$H = -\mu \sum_\alpha N_\alpha - \tfrac{1}{2} \sum_{\alpha,\alpha'} w_{\alpha\alpha'} N_\alpha N_{\alpha'} \tag{56}$$

with

$$N_\alpha = \sum_j n_\alpha(j). \tag{57}$$

[Compare (56) above with the equation following (2) in van Kampen's paper. Although the notation is similar, we should point out that we are using a spinless Fermi lattice-gas description, whereas van Kampen gets his equation from a classical description of a gas of molecules where he neglects the kinetic energy of the individual molecules.]

We can now use our standard techniques to diagonalize the Hamiltonian (56) in terms of temperature-dependent excitations. There is no point to reproduce here the details of the derivation which again is quite similar to those carried on earlier in this paper. We get the following *coupled* equations for the densities in the cells (the reason why the density is uniform within each cell is clarified by the forthcoming discussion)

$$\rho_\alpha(\beta) = \exp\,[\beta\mu'_\alpha(\beta)]/\{1 + \exp\,[\beta\mu'_\alpha(\beta)]\}, \tag{58}$$

$$\mu'_\alpha(\beta) = \mu + \lim \sum_{\alpha'} (w_{\alpha\alpha'},\, \Delta)\rho_{\alpha'}(\beta). \tag{59}$$

This set of coupled equations plays the role of Eqs. (5) in van Kampen's paper. As in van Kempen's treatment, the *uniform* density throughout the total volume (or lattice) is *always* a solution of these equations, and corresponds to the van der Waals isotherms which exist below, as well as above, the critical temperature. This situation corresponds exactly to that of Sec. III, with

$$a = \tfrac{1}{2} \lim \sum_{\alpha'} (w_{\alpha\alpha'},\, \Delta). \tag{60}$$

This also is in agreement with van Kampen's result.

If, moreover, it is assumed that

$$w_{\alpha\alpha'} = w(|\alpha - \alpha'|), \tag{61}$$

then the uniform density, and consequently the van der Waals isotherms, are the *only possible solutions above the critical point.* However, *below* the critical temperature, a nonuniform solution might also be possible, as pointed out by van Kampen; it is a solution which corresponds to the coexistence of *two* phases with different densities, but the same fugacity. This corresponds to the result of Kac and co-workers who obtained, as already stressed, the corresponding Maxwell plateau. For all this part of the argument, the reader is referred to van Kampen's discussion of his Eqs. (5). It is only *before* these equations that our approach differs *significantly* from his. [Moreover, it should also be pointed out that, for a lattice-gas, the introduction of cells is just a superfluous trick, if we want to take the van der Waals limit anyway. Compare, for instance, van Kampen's Eqs. (5) with either (58) and (59), or (26)–(28) of this paper. We indeed introduce this partition into cells just to make more patent the analogy with van Kampen's model. Conversely, van Kampen's model suggests a better insight into the physical meaning of a lattice-gas model.]

There is, however, one case where such a nonuniform density can *never* exist, and this case is precisely given by the Weiss-like models, where not only (61), but also (55) is assumed. This is easily seen by feeding (55) into (59) and then the resulting μ into (58). We hence understand why we found only the van der Waals solutions (see Sec. III). This was due to a defect in the potential, and not in the method. Incidentally, the above discussion also shows why (54) leads to a uniform density within each cell *without* further assumption.

We have then a complete explanation of the apparent discrepancy between Kac's results and ours. Both methods seem to be correct, and ours appears indeed as more general. The difference in the conclusions came from a profound difference between a Weiss-like model, with a space-independent two-body potential, and a Kac-type model, where the two-body interaction is actually space-dependent

(even if this dependence is extremely weak in the van der Waals limit of Kac's potential).

VI. CONCLUSIONS

The models treated in this paper are admittedly rather unrealistic in their extreme schematization of the "intermolecular potential". It should, however, be realized that these simplifications were by no means essential to the applicability of the method; they were indeed chosen just because of the fact that they allow an especially concise presentation of a certain point of view, which, in opposition to the usual treatment of phase transitions, could be summarized as follows.

In the traditional approach (such as Huang's presentation[3] of the Yang and Lee[7] theory), one works within a *fixed* Hilbert space (or phase-space) representation of the system under consideration; one then looks for the analytic properties of the partition function (or rather of its logarithmic derivatives) in the complex fugacity plane. Each domain of analyticity of these objects (determined, in fact, by closed curves of Yang and Lee zeros) which contains at least a segment of the positive real axis, is ultimately associated, in a tentative way, with a separate phase of the system.

Here, on the contrary, one considers, as the principal object of the theory, the algebra generated by, say, the particles field operators. One then considers, for each temperature, the irreducible representations built on the canonical equilibrium state. It turns out that, for certain temperatures (and certain values of the thermodynamical variables), this procedure does not lead to a unique solution. When several solutions coexist, one chooses, as the *normal* physical solution, that which minimizes the corresponding free energy. By sewing together these minimal solutions, one gets the hypersurface of the macroscopic phase space which corresponds to the normal canonical equilibrium states. Outside of this hypersurface, other canonical equilibrium states might be realized which would correspond to the previously disregarded solutions. That these states are really observed depends in last analysis on the very preparation of the system. They, however, always exist as virtual meta-stable states. Hopefully, this point of view could be the germ of a rational introduction, in the frame work of the phase transition problem, of such phenomena as supercooling and superheating.

The method sketched above, and applied to some particular cases in the main body of this paper, was originally suggested by the BCS model for superconductivity. For this model, it describes, in a perhaps not quite familiar language, what is commonly accepted as the correct approach to that specific physical problem. The method was extended here to several systems known to exhibit phase transitions and nonanalytic equations of states, namely a generalized Heisenberg ferromagnet and a generalized lattice-gas. This was done with some detail in order to suggest that the method might be of a more general interest than the BCS model.

It should also be mentioned that the method developed here seems to be just a formalization and, to some extent, an improvement of the ideas presented, from a somewhat more heuristic point of view, by Brout in his monograph.[4]

In closing, we want to make two remarks. First, the limiting procedures considered in the beginning were introduced in an *ad hoc* manner, but their appearance, which is also found in the BCS model, is a natural consequence of the thermodynamical limit itself, when one works in the momentum space rather than in the configuration space. This is one more reason why it is felt that the point of view presented here might be fairly general, even though, for the moment, we only applied it to especially simple models, for obvious didactic reasons.

Second, the reader should realize that the method proposed in this series of papers, in spite of its generality, is to be considered as an exact one to the extend only where the basic assumptions underlying it are valid. For instance, a careful treatment in momentum space of the ordinary Ising model with, say, nearest-neighbor interactions provides an excellent illustration of how careful one should be with these assumptions, and, in particular, with those concerned with the irreducibility of the representations or related concepts. In this case, an assumed irreducibility of the relevant representations would in fact only lead to results known[4] as the Weiss approximation of the Ising model. Another example (namely the BCS theory), in which an abusive irreducibility assumption may generate some difficulties, was already pointed out in a previous paper.[5]

ACKNOWLEDGMENTS

It is a pleasure for the author to acknowledge discussions with Dr. R. H. Brout and with many of his colleagues, of whom special thanks are due to Dr. J. R. Dorfman and Dr. E. W. Montroll for several fruitful conversations, as well as to Dr. M. S. Green and Dr. R. Zwanzig for their active participation in a seminar held on the topics presented in this manuscript.

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High-Energy Behavior of Feynman Integrals with Spin. II

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The analysis of a previous paper is applied to determine the leading behavior and coefficients of specific lower-order terms of planar graphs in the nucleon–meson scattering process. The results of Cheng and Wu in verifying the Reggeization hypothesis in sixth order are rederived and a method of extending the analysis to nth order is indicated.

INTRODUCTION

IN an earlier paper[1] (hereafter referred to as I) we outlined a general method for determining the leading behavior at large values of the momentum transfer t of any Feynman integral F_G corresponding to a planar graph G in any two-body process in a conserved vector theory describing the interaction of a spin-$\frac{1}{2}$ nucleon with a spin-1 meson. The method hinged on the concept of straddling. Straddling is defined with respect to specific subgraphs of G, or, in the terminology of I, certain scaling sets of G. For analysis of leading behavior, we are concerned only with those scaling sets S_1 that

(i) contain at least one t path[1,2];

(ii) are such that no two external lines of the set are one and the same line;

(iii) are such that if l_i is any loop of the graph not belonging to the scaling set then there is a partition[1] from loop l_i to that part of the boundary of the graph joining the vertices of either the incoming or outgoing particles that does not cut any line of the scaling set; and

(iv) do not contain any line that when cut separates the scaling set into two parts and at the same time does not belong to any t path lying entirely within the scaling set.

Sets not satisfying (i), (ii), (iii), and (iv) are always unimportant in determining the leading behavior. A scalar product $X_i \cdot X_j$, where[1] $X_i = (1/2C)(\partial D/\partial b_i)$ and C and D are the well-known Chisholm determinants[3,4] straddles such a scaling set S_1 only if all partitions from loop l_i to loop l_j cut at least one line of S_1 when $i \neq j$. If $i = j$ then the scalar product $X_i \cdot X_i$ straddles the set if the loop l_i belongs to the set. If $r(l)$ is the number of lines (loops) in the set S_1 and β is the maximum number of straddling scalar products that can be formed, then we say that the set S_1 generates a t^α behavior, where $\alpha = 2l + \beta - r$. If α_1 is the maximum value of α over the set of scaling sets satisfying the four conditions stated above, then the leading behavior of the graph G is $t^{\alpha_1} \ln^b t$, where b is a positive integer, a function of G. For the meson–meson scattering process[1] the sets generating the t^{α_1} behavior are easily characterized. All sets satisfying the four conditions stated above together with the condition that all external lines of the set are meson lines generate the leading behavior of t^2. b is just the number of such sets consistent with certain constraints explicitly stated in I. The existence of divergent subgraphs in the graph G renders the prescription for the leading behavior more complicated.

In this paper we wish to characterize these maximal sets for the other two-body processes. In Sec. 1 we analyze the general planar graph for the nucleon–meson scattering process and determine α_1 as zero. In Secs. 2 and 3 we consider the ladder graphs for this process and explicitly locate those parts of the Feynman integral that contribute to the leading behavior and certain lower-order terms. In Sec. 4 we consider the general planar graph for the other two-body processes.

As in I the external particles are labeled by the index i, $i = 1, 2$ corresponding to the incoming particles and $i = 3, 4$ corresponding to the outgoing particles. The ith external particle has momentum p_i. Further, we denote the boundary joining external-particle vertices i and j by b_{ij}; it is along $b_{12}(b_{34})$ that we run momentum $p_1(p_4)$ and along b_{23} that we run momentum $p \equiv p_1 + p_2$. In the specific case of the meson–nucleon ladder graph we

* This work is supported in part through funds provided by the Atomic Energy Commission Contract AT(30-1)-2098.
[1] J. V. Greenman, J. Math. Phys. 7, 1782 (1966).
[2] G. Tiktopoulos, Phys. Rev. 131, 480, (1963).
[3] J. S. R. Chisholm, Proc. Cambridge Phil. Soc. 48, 300 (1952).
[4] R. J. Eden, Phys. Rev. 119, 1763, (1960).

break our rule and run momentum p along a different path.

A nucleon path of the graph is called an open (closed) nucleon path if that path contains (does not contain) external nucleon lines of the graph.

Further, for ease of discussion, we often fail to distinguish between a set of Feynman parameters and the corresponding set of lines in the graph.

We denote the mass of the nucleon (meson) by $m_1(m_2)$ and throughout we use the metric $g_{00} = -g_{11} = -g_{22} = -g_{33} = 1$.

1. GENERAL PLANAR GRAPH IN THE NUCLEON–MESON SCATTERING PROCESS

For the first part of the analysis we do not restrict ourselves to the nucleon–meson scattering process. We consider some two-body planar graph G and the corresponding Feynman integral F_G in the form first derived by Chisholm,[3] where F_G is expressed as an integral over the Feynman parameters of a sum of terms, the sum being denoted by I_G^2 and expressed as

$$\sum_{i=0}^{[\frac{1}{2}r_n]} A_i C^{r-2l-2-i} D^{-(r-2l-i)}, \tag{1.1}$$

where $[\frac{1}{2}r_n]$ denotes the highest integer not greater than $\frac{1}{2}r_n$, and A_i are coefficients that are functions of the external momenta and masses of the system and the derivatives

$$X_i = \frac{1}{2C}\frac{\partial D}{\partial b_i}, \qquad X_{ij} = \frac{1}{8C}\frac{\partial^2 D}{\partial b_i\,\partial b_j}$$

extensively studied in I. The problem of determining the leading behavior of F_G is equivalent to that of determining the maximum number of scalar products that can be formed that straddle any scaling set that belongs to the set of scaling sets satisfying the four conditions stated in the Introduction.

Suppose such a set S contains r lines, l loops, n vertices, e_m external meson lines and e_n external nucleon lines, i_m internal meson lines and i_n internal nucleon lines, then the following relations are true,

$$\begin{aligned} r &= 3(l-1) + (e_m + e_n), \\ n &= 2(l-1) + (e_m + e_n), \\ i_n &= 2(l-1) + e_m + \tfrac{1}{2}e_n, \\ i_m &= (l-1) + \tfrac{1}{2}e_n. \end{aligned} \tag{1.2}$$

Suppose further that the set S divides the graph G into three distinct, disjoint, connected regions—the subgraph S itself and region $R_1(R_4)$ having part of its boundary in common with $b_{12}(b_{34})$.

To calculate the number of straddling scalar products, we need to know now many $p_1(p_4)$ momenta from region $R_1(R_4)$ can be paired with $p_4(p_1)$ momenta from S or $R_4(S$ or $R_1)$. These momentum scalar products are generated

(i) in trace and helicity inner product calculations;
(ii) by means of meson line $g_{\mu\nu}$ factors;
(iii) by means of $X_{ij}g_{\mu\nu}$ factors.

We first outline four methods of simplifying products of γ-matrices.

Method I. Any product of γ-matrices can be written as a linear sum over the 16 linearly independent matrices of the Dirac algebra.[5] For instance, an odd product can be written as a sum over the eight matrices γ_ν, $\gamma_5\gamma_\nu$.

Explicitly,

$$\gamma_{\mu 1}\cdots\gamma_{\mu_{2n+1}} = a^\nu_{\mu_1\cdots\mu_{2n+1}}\gamma_\nu + b^\nu_{\mu_1\cdots\mu_{2n+1}}\gamma_5\gamma_\nu, \tag{1.3}$$

where the coefficients are given by

$$a^\nu_{\mu_1\cdots\mu_{2n+1}} = +\tfrac{1}{4}\,\mathrm{Tr}\,(\gamma_{\mu_1}\cdots\gamma_{\mu_{2n+1}}\gamma^\nu), \tag{1.4}$$

$$b^\nu_{\mu_1\cdots\mu_{2n+1}} = -\tfrac{1}{4}\,\mathrm{Tr}\,(\gamma_{\mu_1}\cdots\gamma_{\mu_{2n+1}}\gamma_5\gamma^\nu). \tag{1.5}$$

Method II. If there occurs in a product of γ-matrices the pair γ^μ, γ_μ with an odd number of γ-matrices between, we can exploit the formula[6]

$$\gamma^\mu\gamma_{\mu_1}\cdots\gamma_{\mu_{2n+1}}\gamma_\mu = -2\gamma_{\mu_{2n+1}}\cdots\gamma_{\mu_1}. \tag{1.6}$$

Method III. Whenever momentum p_1 or p_4 is associated[1] with adjacent γ-matrices in a product then we can no longer use these momenta to form scalar products $(p_1\cdot p_4)$, since we know the relations

$$(\gamma\cdot p_1)(\gamma\cdot p_1) = p_1^2, \tag{1.7}$$

$$(\gamma\cdot p_4)(\gamma\cdot p_4) = p_4^2, \tag{1.8}$$

are true. If p_1 and p_4 are alternately associated with γ-matrices in a product of γ-matrices then we can use the relation

$$\begin{aligned}(\gamma\cdot p_1)(\gamma\cdot p_4)(\gamma\cdot p_1) \\ = -m_1^2(\gamma\cdot p_4) + 2(p_1\cdot p_4)(\gamma\cdot p_1).\end{aligned} \tag{1.9}$$

Method IV. Finally, we outline the method introduced by Gell-Mann *et al.*[7] and extensively used by Polkinghorne[8] of simplifying helicity inner products. Suppose $u_4(u_1)$ is the helicity spinor of $p_4(p_1)$; then to calculate

$$[\bar{u}_4(\gamma\cdot A_1)\cdots(\gamma\cdot A_i)(\gamma\cdot p_1)(\gamma\cdot A_{i+1})\cdots(\gamma\cdot A_n)u_1] \tag{1.10}$$

[5] S. S. Schweber, *Introduction to Relativistic Quantum Field Theory* (Harper & Row, Publishers Inc., New York, 1961).
[6] H. Cheng and T. T. Wu, Phys. Rev. **140**, B465 (1965).
[7] M. Gell-Mann, M. L. Goldberger, F. E. Low, E. Marx, and F. Zachariasen, Phys. Rev. **133**, 145 (1962).
[8] J. C. Polkinghorne, J. Math. Phys. **5**, 1491 (1964).

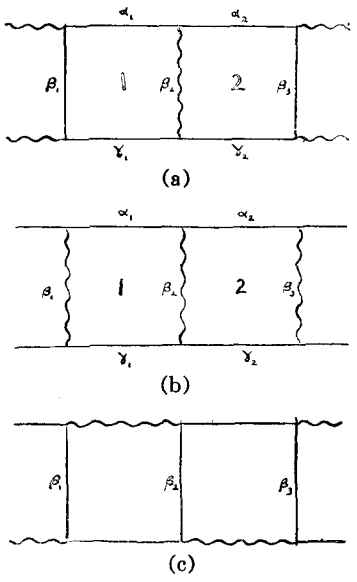


FIG. 1. Application of the leading behavior formula.

we move $(\gamma \cdot p_1)$ to the right using the anticommutation relations of the γ-matrices and annihilate[8] $(\gamma \cdot p_1)$ against the helicity spinor using the relation $(\gamma \cdot p_1)u_1 = m_1 u_1$. Similarly, we would move $(\gamma \cdot p_4)$ to the left. The method is not limited just to the spinors u_1, u_4 since we can effectively annihilate $p_1(p_4)$ against $u_2(u_3)$ using the following relations:

$$(\gamma \cdot p_1)u_2 = (\gamma \cdot p)u_2 - m_1 u_2, \tag{1.11}$$

$$(\gamma \cdot p_4)u_3 = (\gamma \cdot p)u_3 - m_1 u_3. \tag{1.12}$$

The first term on the right-hand side obviously cannot be used to generate straddling scalar products.

For each section of those nucleon paths having nonzero intersection with S—the sections being defined by the intersection of the path with S—we reduce the corresponding product of γ-matrices in I_G^2 by method I. Simplification of the resulting traces is effected by methods II and III. It is now straightforward to evaluate the maximum number of X_i functions that can form straddling scalar products. Suppose for a specific term of the Chisholm expansion, $i_n'(2i_n'')$ is the number of nucleon lines of the set S that together with nucleon lines in either region R_1 or R_4 (region S) generate X_{ij} functions. Suppose further that w is the total number of sections of all those nucleon loops of G with nonzero intersection with S that do not lie in S. Suppose finally that for the ith of the k open nucleon paths of G with nonzero intersection with S there are s_i sections that do not lie in S but whose end vertices both belong to S and that for k' of these k open nucleon lines both external nucleons of the open nucleon path are either incoming or outgoing. The number of X_i functions that can form straddling scalar products consists of the $(i_n - i_n' - 2i_n'')X_i$ functions from the nucleon lines of S, together with the $(e_m + i_n')X_i$ functions paired by the external meson lines of S and the $X_{ij}g_{\mu\nu}$ functions, together with the $(w + \Sigma s_i + k')X_i$ functions from those sections of the nucleon loops and open nucleon paths not lying in S. In addition we have $i_n''X_{ij}$ functions where l_i and l_j both lie in S. These functions are effective straddling scalar products as explained at length in I. Any scalar product paired by an $X_{ij}g_{\mu\nu}$ factor, where $l_i(l_j)$ lies in $R_1(R_4)$, does not straddle S even if the $p_1(p_4)$ momentum is contributed by a nucleon line in $R_1(R_4)$ since, on scaling, this X_{ij} function behaves as ρ, where ρ is the scaling parameter for set S.

The maximum number of X_i functions that can form straddling scalar products is therefore $(i_n + e_m + w + \Sigma s_i + k')$. Since $\frac{1}{2}e_n = k + \Sigma s_i + w$, the set S generates a leading behavior of $2 - \frac{1}{2}e_n - [\frac{1}{2}(k - k')]$, where the square bracket indicates the smallest integer not smaller than $\frac{1}{2}(k - k')$. As an example let us consider the graph of Fig. 1(a). Meson line β_2 generates a t^0 behavior with one straddling scalar product whereas nucleon line β_1 generates a t^1 behavior with two straddling scalar products. Loop 1 also generates a t^1 behavior. In the example of Figure 1(b) the sets β_1, β_2, β_3 all generate a t^{-1} behavior with no straddling scalar product. In the example of Fig. 1(c), the sets β_1, β_2, β_3 all generate a t^0 behavior with one straddling scalar product.

For any planar graph G for the nucleon–meson scattering process the leading behavior is at most $t^0 \ln^b t$, where b is some positive integer, a function of G. The sets that generate this behavior satisfy the four conditions specified in the Introduction together with the constraint $e_n = 2$. But these conditions are not sufficient to characterize these sets. To specify the additional constraints, we need to introduce additional notation.

(i) Let us label the only section of the open nucleon path lying in S as section A and the corresponding product of γ-matrices in I_G^2 as X.

(ii) Let us label the first (last) vertex of section A traveling along the nucleon path as $a_1(a_{2p+1})$.

(iii) Let us define a $p_1(p_4)$ vertex as a vertex common to section A and an external meson line of S lying in the region $R_1(R_4)$.

(iv) Let us define an m-line of S as a nucleon line of section A that when cut separates S into two parts.

(v) Let us denote the matrix X, after the elimination of the γ_μ, γ^μ pairs by Method II, by X^1.

We note first that if X^1 is a product of $2q$ or $(2q + 1)$ γ-matrices we can only generate the leading behavior of t^0 for the set S if q of these γ-matrices are associated[1] with p_1 and q with p_4. Hence one nucleon line of section A could provide a p momentum or an m_1 factor. Alternatively one vertex could fail to provide a p_1 or p_4 momentum.

Secondly, we note that all m-lines, except possibly one m-line which would provide an m_1 factor or momentum p for example, must provide a p_1 or p_4 momentum. They cannot generate X_{ij} factors since there would be no partition from loop l_i to loop l_j lying entirely in the set S. Further, consecutive m-lines of section A, if they provide p_1, p_4 momenta, must both provide either p_1 or p_4 momenta, provided that no nucleon line in that section of section A lying between the consecutive m-lines contributes an m_1 factor or momentum p since otherwise corresponding to this section in the matrix X^1 there is an odd product of γ-matrices alternately associated with p_1 and p_4. Hence in traveling along that section of the open nucleon path lying in S there can be only one occasion on which a $p_1(p_4)$ vertex of an m-line follows a $p_4(p_1)$ vertex of an m-line. For example, in Fig. 2 the rungs AB, EF generate a t^0 behavior whereas CD generates a t^{-1} behavior.

Thus for a scaling set to generate a t^0 behavior it must satisfy the four conditions specified in the introduction together with the following two conditions that

(v) the set contains only two external nucleon lines;

(vi) in traveling along that section of the open nucleon path lying in S there can be only one occasion on which a $p_1(p_4)$ vertex of an m-line follows a $p_4(p_1)$ vertex of an m-line.

In I we determined the leading behavior of divergent terms in the Chisholm expansion by explicit renormalization. For the planar meson–meson scattering graphs the leading behavior of the complete Feynman integral is often greater than that determined by simple power counting methods if there exist divergent subgraphs. Similarly for divergent planar nucleon–meson graphs the leading behavior is often greater than that determined by power counting. For the graph of Fig. 3(c), for example, the leading behavior is one power of ln t greater than that determined by power counting. For the graph of Fig. 3(a), however, power counting gives us the correct leading behavior.

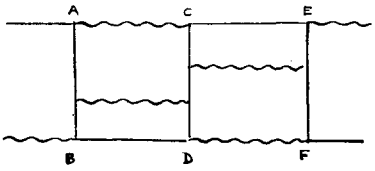


FIG. 2. Scaling sets for a meson–nucleon scattering graph.

We now determine the leading behavior of the graph of Fig. 3(a) as an example of the general analysis of this section. Following Gell-Mann *et al.*[7] we use gauge freedom to replace the γ-matrix for the external meson vertex (2) by the matrix $\Gamma^2_\mu \equiv \gamma_\mu - p_{3\mu}(\gamma\cdot p_2)(p_2\cdot p_3)^{-1}$ and for the external meson vertex (3) by $\Gamma^3_\mu = \gamma_\mu - p_{2\mu}(\cdot p_3)(p_2\cdot p_3)^{-1}$. Whatever the polarization vectors, all the anticommutators $\{\Gamma^i_\mu, \gamma\cdot p_1\}$, $\{\Gamma^i_\mu, \gamma\cdot p_4\}$ are at most constant at large values of t. We thus say that the external vector meson vertices are inactive in that they cannot couple polarization vectors in any way to form scalar products proportional to t.

Using the general results of this section it is evident that there are three possible t^0 scaling sets, (β_4), (β_1, β_3), $(\beta_3$, loop 1). If it were not for renormalization, the t^0 ln ^2t behavior would derive solely from the basic term of the Chisholm expansion for the simple reason that if (β_1, β_3) is to be a scaling set there must be two distinct scalar products straddling that set. In Fig. 3(a) we indicate which nucleon lines provide the p_1 and which the p_4 momentum to generate maximum behavior in the basic term; an arrow to the left (right) adjacent to a nucleon line indicates that that line contributes a $p_1(p_4)$ momentum.

The divergent part of the second term of the Chisholm expansion when renormalized has a leading behavior of t^0 ln ^2t. Combining the two contributions we find that the Feynman integral for the graph of Fig. 3(a) has a leading behavior of

$$(-1)(t^0 \ln^2 t)H, \tag{1.13}$$

where we define H as

$$\int_0^1 \int_0^1 d\alpha\, d\beta\, \delta(\alpha + \beta - 1) \times \Gamma^3_\mu[(1-\alpha)(\gamma\cdot p) + m_1]\Gamma^2_\nu h'^{-1}, \tag{1.14}$$

where h' is the D function for the two-line bubble. Similarly we can determine the behavior of the Feynman integral for the graph of Fig. 3(b). We find it equal to (1.13).

The argument is not identical for the graph of Fig. 3(c). The basic term of the Chisholm expansion does not have a leading behavior of t^0 ln ^2t. This can

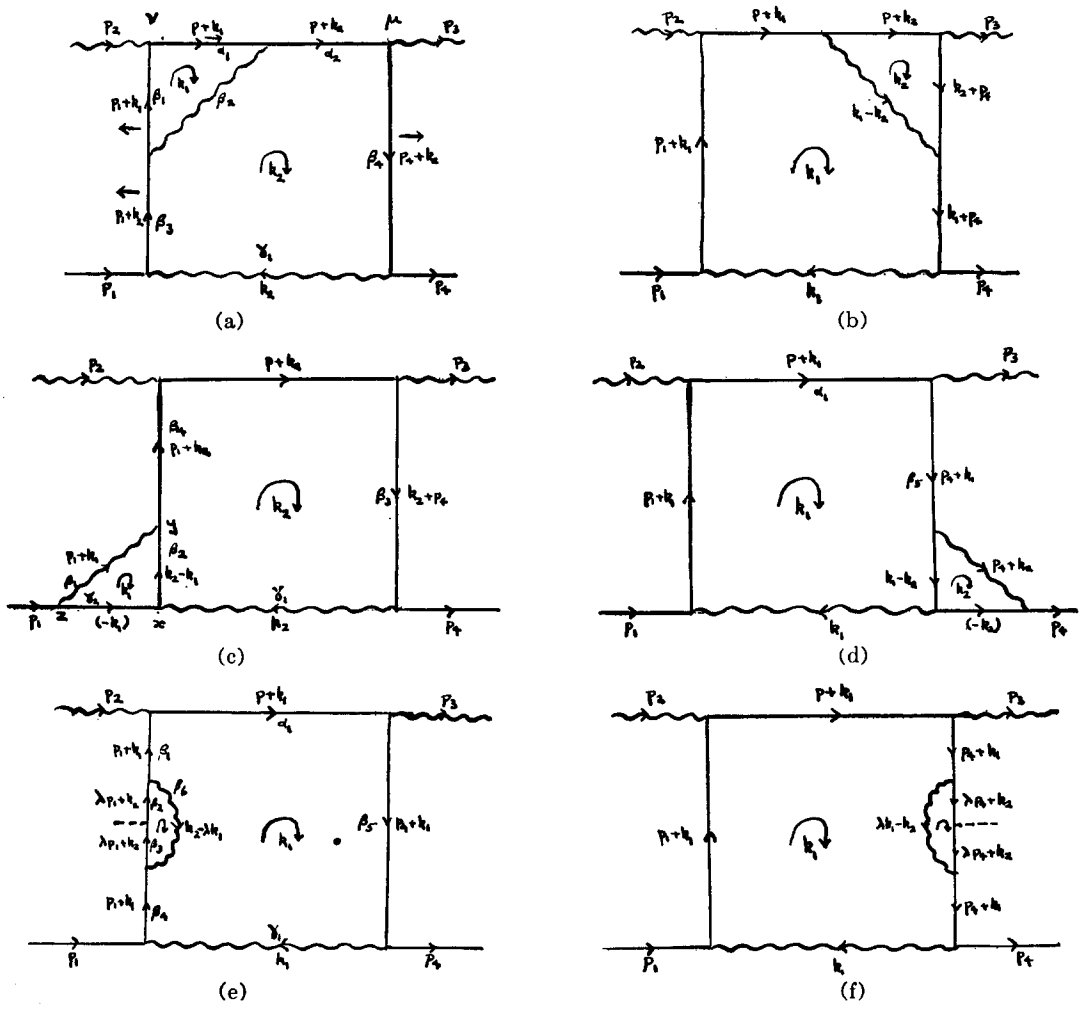


FIG. 3. Examples of divergent graphs.

be seen most easily by moving the p_4 momentum of β_3 to vertex x. Both nucleon lines β_2 and γ_2 must then provide p_1 momenta since otherwise we would lose a straddling scalar product. Eliminating the γ_μ, γ^μ pair of vertices y and z by method II we find that necessarily $\gamma \cdot p_1$ multiplies the spinor for the incoming nucleon, and since the Γ vertex is inactive there can only be at most one scalar product straddling the set (β_2, β_4). (β_2, β_4), therefore, is no longer a t^0 scaling set.

The $t^0 \ln {}^2t$ behavior derives solely from the renormalized part of the second term of the Chisholm expansion. Simple integration yields the leading behavior of the Feynman integral of Fig. 3(c) as

$$(+1)(t^0 \ln^2 t)H. \tag{1.15}$$

Similarly the leading behavior of the Feynman integral of Fig. 3(d) is

$$(+1)(t^0 \ln^2 t)H. \tag{1.16}$$

The $t^0 \ln {}^2t$ behavior therefore cancels in the sum of the four graphs Fig. 3(a)–(d).

Let us now determine the leading behavior of the graph of Fig. 3(c). A procedure was outlined in I and we follow that procedure in this calculation. We use the Ward method and introduce a zero momentum meson vertex in the nucleon self-energy part together with an integration over a new "Feynman parameter" λ. The leading behavior derives solely from the divergent part of the second term of the Chisholm expansion. The important part of this divergent term is

$$(-4t) \int_0^1 d\lambda \int_0^1 \prod_{i=1}^{8} d\alpha_i C\, D^{-3} X_{22}(p_1 \cdot X_1) \times \delta\Big(\sum_{i=1}^{8} \alpha_i - 1\Big) Q, \tag{1.17}$$

where

$$Q = \Gamma_\mu^3[(1 - \alpha_1)(\gamma \cdot p) + m_1]\Gamma_\nu^2.$$

Renormalized, the leading term can be written

$$(+4t^3)\int_0^1 d\lambda \int_0^1 d\bar{\beta}_1 \int_0^1 d\bar{\beta}_2 \int_0^1 d\bar{\beta}_3 \times \delta(\bar{\beta}_1+\bar{\beta}_2+\bar{\beta}_3-1) \times \int_0^1 d\beta_4 \int_0^1 d\beta_5 \int_0^1 d\beta_6 \int_0^1 d\alpha_1 \int_0^1 d\gamma_1 \int_0^1 dp \times \delta(\beta_4+\beta_5+\beta_6+\alpha_1+\gamma_1+p-1) \times \int_0^1 d\chi \frac{C_1(-3)\lambda^2(\bar{\beta}_1+\bar{\beta}_2)\bar{\beta}_3\beta_6^2 Q}{[[\lambda^2(\beta_1+\beta_2)\beta_3\beta_6 p\chi+(\beta_4+\beta_5)\beta_6]t+h]^4}. \tag{1.18}$$

The leading behavior is then obtained using the formula of Tiktopoulos[2] as

$$(-4)(t^0 \ln^2 t)H \int_0^1 d\lambda \int_0^1 d\bar{\beta}_1 \int_0^1 d\beta_2 \int_0^1 d\bar{\beta}_3 \times \delta(\bar{\beta}_1+\bar{\beta}_2+\bar{\beta}_3-1) \int_0^1 d\beta_4 \int_0^1 d\beta_5 \int_0^1 d\chi \times \frac{\lambda^2(\bar{\beta}_1+\bar{\beta}_2)\bar{\beta}_3\,\delta(\beta_4+\beta_5+\chi-1)}{[\lambda^2(\beta_1+\beta_2)\beta_3\chi+(\beta_4+\beta_5)]^3}. \tag{1.19}$$

The integrations are trivial. The leading term is simply

$$(-1)(t^0 \ln^2 t)H. \tag{1.20}$$

The sum of the Feynman integrals for the six graphs 3(a)–3(d) has a leading behavior of

$$(-2)(t^0 \ln^2 t)H. \tag{1.21}$$

2. LEADING TERMS FOR THE LADDER GRAPHS IN THE NUCLEON-MESON SCATTERING PROCESS

A. Three-Rung Ladder

This graph has already been considered by Cheng and Wu.[6] We rederive their results using our methods. We again replace the γ-matrices for the external meson vertices by the Γ matrices, defined in the previous section. The general analysis of the previous section indicates that there are five t^0 scaling sets, the over-all delta function only permitting us to scale four. The possible sets of scaling sets are $(\beta_1, \beta_2, \beta_3, l_2)$ and $(\beta_1, \beta_2, \beta_3, l_1)$ in the notation of Fig. 4(a). For β_1 and β_3 to be possible scaling sets we must ensure that there exists a scalar product straddling each of these sets. The only way we can achieve this is for nucleon line $\beta_1(\beta_3)$ to contribute an explicit[8] $p_1(p_4)$ momentum. These momenta must be transported by the meson lines α_1, α_2 to vertices A, B. If l_2 is to be a scaling set then there must be two scalar products straddling l_2. Neither γ_2 nor β_2 can contribute either a p_1 vector or p_4 vector, for that would imply two adjacent γ-matrices associated with the same momentum vector. Hence the p_1 vector from β_1 must be paired with the p_4 vector from β_3 and the nucleon lines β_2, γ_2 must generate an X_{22} factor. (For the second set of scaling sets nucleon lines γ_1 and β_2 would generate an X_{11} factor.)

For the first set the leading behavior of $t^0 \ln {}^3t$ derives from those terms of the original integrand I_G^1 that contain the momentum scalar products

$$(p_1\cdot p_4)(k_2\cdot k_2),\ (p_1\cdot k_2)(k_2\cdot p_4). \tag{2.1}$$

For the second set the corresponding scalar products are

$$(p_1\cdot p_4)(k_1\cdot k_1),\ (p_1\cdot k_1)(k_1\cdot p_4). \tag{2.2}$$

The second terms in (2.1) and (2.2) do not in fact contribute[8] to the $t^0 \ln {}^3t$ behavior. We prove this in Appendix A.

B. The n-Rung Ladder

In the case of the three-rung ladder we can characterize the sets of scaling sets by which one of the two nucleon lines that are not rungs of the ladder are inactive in the sense that their momenta are not used to generate straddling scalar products. In the

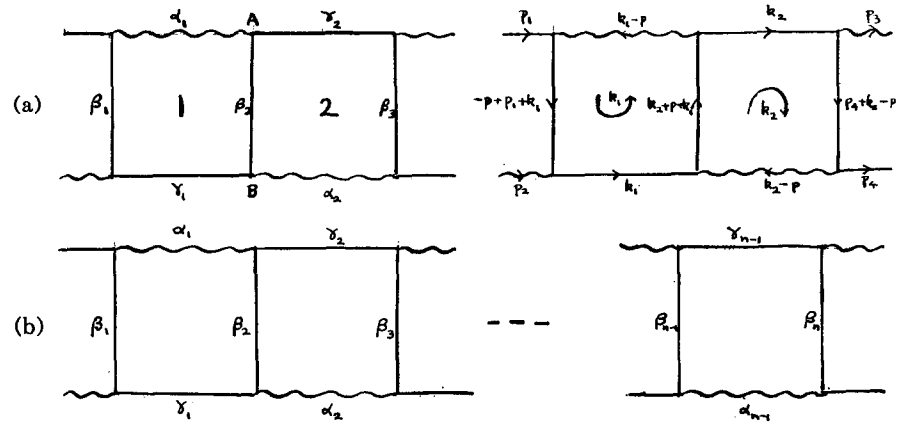


FIG. 4. The ladder graphs.

same way we can characterize the sets of scaling sets for the n-rung ladder by which of the nucleon lines $\gamma_i (i = 1, \cdots, n-1)$—in the notation of Fig. 4(b)—are inactive. With nucleon line γ_1 inactive one possible set of scaling sets is $\beta_1, \beta_2, \cdots, \beta_n, l_2, l_3, \cdots, l_n$. The p_1 momentum of β_1 must be paired with the p_4 momentum of β_n and the lines of β_i, γ_i generate X_{ii} factors $(i = 2, \cdots, n)$. The fact that the explicit p_1 and p_4 momenta must be paired is immediate, for if instead we formed the product $(p_1 X_i)(X_i X_l)$ or $(p_1 X_i)(X_i p_4)$ then the X_i factors must be contributed by the rungs β_i and β_{i+1}. Thus the nucleon line γ_i is either rendered inactive or γ_i generates an X_{ij} factor with another line. i cannot be equal to one and hence in the first case with two inactive lines the leading behavior is necessarily lowered. In the second case, since $i \neq j$ either β_i or β_{i+1} is no longer a t^0 scaling set.

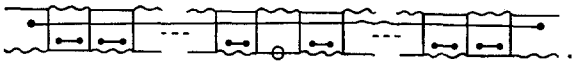
Again, when $\gamma_p (p \neq 1, p \neq n-1)$ is inactive the explicit momenta p_1, p_4 of β_1, β_n must be paired. With $\gamma_p (1 \leq p \leq n-1)$ inactive the leading behavior derives from those terms of the integrand I_G^1 whose numerator is constructed out of the momenta p_1, p_4 and the pairs k_i, $k_i (1 \leq i \leq n-1, i \neq p)$.

Theorem: It is only that part of I_G^1 with the product

$$(p_1 \cdot p_4) \prod_{\substack{i=1 \\ i \neq p}}^{n-1} k_i^2$$

as numerator that contributes to the leading behavior of $t^0 \ln^{2n-3} t$ with γ_p inactive.

The proof is given in Appendix A. There are therefore $(n-1)$ terms of the original integrand that contribute to the leading behavior of $t^0 \ln^{2n-3} t$, corresponding to each of those nucleon lines that are not rungs being inactive. If we represent each scalar product $(k_i \cdot k_j)$ by the partition between l_i and l_j, where we define $k_0 (k_n)$ as $p_1 (p_4)$ and $l_0 (l_n)$ as the area defined by the external particle lines 1 and 2 (3 and 4), and if we denote each inactive nucleon line by a circle on that line, then we can represent these $(n-1)$ terms by the diagrams



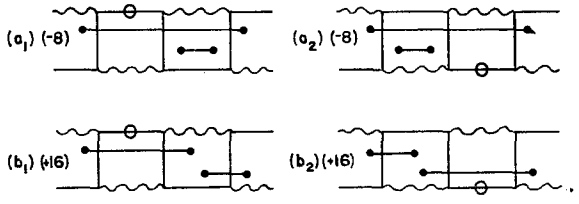
3. LOWER-ORDER TERMS FOR THE LADDER GRAPHS IN THE NUCLEON-MESON SCATTERING PROCESS

The second-order term of the Feynman integral for the three-rung ladder is a sum of the leading order parts of those terms of the Chisholm expansion that have a leading behavior of $t^0 \ln^2 t$ together with the second-order parts of those terms of the Chisholm expansion that have a leading behavior of $t^0 \ln^3 t$. These latter contributions are difficult to calculate explicitly. However, in the Reggeization problem the calculations do not have to be performed because there is cancelation of the complete terms of I_G^1 having leading behavior—not just the leading-order parts of these terms—by terms derived from certain nonplanar graphs. This is the reason why it is advantageous to revert to the study of the integrand I_G^1 once we have determined by our analysis the leading behavior and which terms in the Chisholm expansion contribute to the leading behavior and lower-order behavior. When we are concerned with cancellation we revert to study of I_G^1; when we wish to determine the coefficient of the leading order of a sum of terms of the Chisholm expansion (I_G^2) all with the same leading behavior we always calculate in the Chisholm form where the p_1, p_4 momenta are still associated with γ-matrices and are not yet paired to form scalar products. Method III then considerably simplifies the analysis.

Let us illustrate these points by now explicitly calculating the second-order terms for the three-rung ladder.

A. Lower-Order Contributions from Terms with Leading Behavior of $t^0 \ln^3 t$

There are two sets of these terms:



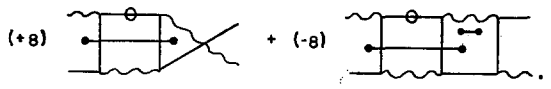
We prove in Appendix A that although there are $t^0 \ln^3 t$ terms in the Chisholm expansion of $(b_1)(b_2)$ there is complete cancellation of the $t^0 \ln^3 t$ behavior between these terms. However, we consider $(b_1)(b_2)$ under this heading since the $t^0 \ln^2 t$ terms of $(b_1)(b_2)$ are part of the second-order part of that term of the second term of the complete Chisholm expansion (I_G^2) that has a leading behavior of $t^0 \ln^3 t$.

We find in the third paper of this series (and as already shown by Polkinghorne[8] and Cheng and Wu[6]) that the complete terms $(a_1)(a_2)$ are canceled by contributions from certain nonplanar graphs.

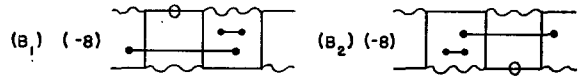
Both (b_1) and (b_2) have a leading behavior of $t^0 \ln^2 t$ and we can exhibit this fact by using the relation

$$\tfrac{1}{2}(p_4 + k_2)^2 = \tfrac{1}{2} m_1^2 + \tfrac{1}{2} k_2^2 + (p_4 \cdot k_2). \qquad (3.1)$$

We then rewrite (b_1) as



The first term has a leading behavior of t^0; the second term a leading behavior of $t^0 \ln^2 t$. We show in the third paper that the terms



are exactly canceled by contributions from certain nonplanar graphs.

B. Terms with Leading Behavior of $t^0 \ln^2 t$

We denote terms of the Chisholm expansion (I_G^2) by superimposing the following symbols on the graph G:

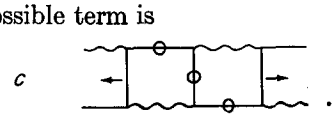
(i) An arrow to the left (right) adjacent to a nucleon line indicates that that nucleon line contributes a $p_1(p_4)$ momentum. If the arrow lies in loop k_i the momentum is contributed by X_i.

(ii) A circle on a nucleon line indicates that that line contributes a p momentum or m_1 factor.

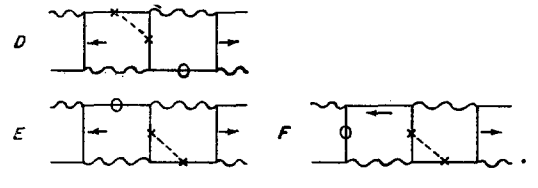
(iii) A cross on a nucleon line indicates that that line generates an X_{ij} factor with another nucleon line. The pairing is indicated by a dotted line joining the two crosses.

We consider the $t^0 \ln^2 t$ terms under three headings:

(a) *Terms with scaling sets* $\beta_1\beta_2\beta_3$
The only possible term is

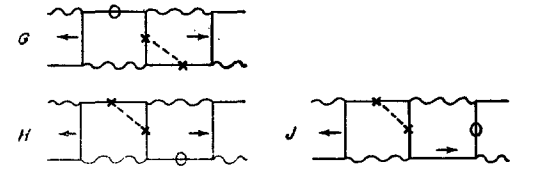


(b) *Terms with scalings sets* $\beta_2\beta_3 l_2$ *and* $\beta_2\beta_3 l_1$
These terms have the structure



Terms E and F are canceled by terms from certain nonplanar graphs.

(c) *Terms with scaling sets* $\beta_1\beta_2 l_1$ *and* $\beta_1\beta_2 l_2$
These terms have the structure



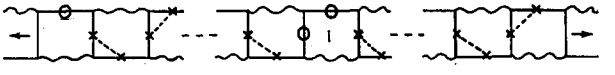
Terms H and J are canceled by terms from certain nonplanar graphs.

(d) *Terms with scaling sets* $\beta_1\beta_3 l_2$ *and* $\beta_1\beta_3 l_1$
There can be no such terms since we can only form at most two scalar products in the numerator of I_G^1. The sum of the leading behavior of terms D and G is

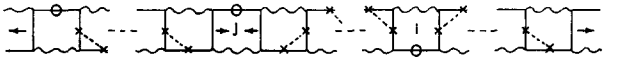
$$(+2)(t^0 \ln^2 t)H.$$

The leading behavior of the sum of graphs Fig. 3(a)–(f) and Fig. 4(a) together with the two nonplanar graphs studied in the work of Refs. 6 and 8 is simply the leading behavior of C, the term required for verification of the Reggeization hypothesis in the sixth order.

Similarly for the n-rung ladder contributions to the $t^0 \ln^{2n-4} t$ behavior from those terms with leading behavior $t^0 \ln^{2n-4} t$ are most simply calculated in the Chisholm form. For instance, the term with $t^0 \ln^{2n-4} t$ behavior that has γ_i inactive and does not have loop l_i as a scaling set must have either the structure

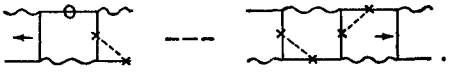


or the structure



For either of these terms the coefficient of $t^0 \ln^{2n-4} t$ is immediately obtainable from the integration formula of Tiktopoulos.[2]

Similarly we can determine those terms that have a leading behavior of $t^0 \ln^{2n-4} t$ with γ_i inactive and β_n not a t^0 scaling set. There can be only one configuration:



We study the planar n-rung ladder in detail in the third paper of this series.

4. HIGH-ENERGY BEHAVIOR OF OTHER TWO-BODY SCATTERING PROCESSES

A. Nucleon–Nucleon Scattering in the s Channel

The analysis of Sec. 1 has shown that any planar graph in the nucleon–nucleon scattering process can have at most a leading behavior of $t^{-1} \ln^b t$.

The t^{-1} scaling sets are easily characterized. They must satisfy the conditions (i)–(vi) together with the amended fifth condition that

(v′) the t^{-1} scaling set contains only four external nucleon lines. As we have seen, for the graph of

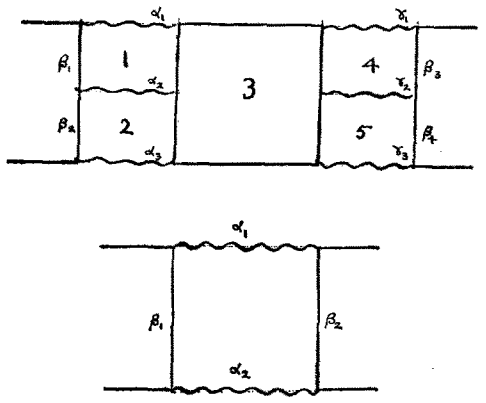


FIG. 5. Nucleon–antinucleon leading behavior.

Fig. 1(b) there are five t^{-1} scaling sets $-\beta_1$, β_2, β_3, loop 1, and loop 2. Delta-function constraints permit us to scale only four of these sets at any one time.

B. Nucleon–Antinucleon Scattering in the s Channel

This is essentially the meson–meson scattering process. The leading behavior for any planar graph for nucleon–antinucleon scattering is at most $t^2 \ln^b t$. This maximum is achieved for graph G if there exists a subgraph of G satisfying the four conditions stated in the Introduction together with the condition that there are no external nucleon lines to the subgraph and provided there is a term of the Chisholm expansion for which all external meson lines of the scaling set can generate distinct straddling scalar products. That this last proviso can always be satisfied is obvious for all sets except those sets whose $p_1(p_4)$ meson lines[1] connect to a complete open nucleon path connecting the two incoming (outgoing) particles, as, for example, in the case of the graph depicted in Fig. 5(a). This graph has a leading behavior of t^2 with loop 3 the t^2 scaling set if all three meson lines $\alpha_1\alpha_2\alpha_3(\gamma_1\gamma_2\gamma_3)$ convey $p_1(p_4)$ momenta from the open nucleon paths to loop 3. That there exists a term in the Chisholm expansion for which this is true follows immediately from Eq. (B13) of Appendix B.

If there exists no subgraph S_1 with no external nucleon lines then the behavior is necessarily at most $t^1 \ln^b t$. For instance, for the graph of Fig. 5(b) there are two t^1 scaling sets—β_1, β_2—each with two straddling scalar products, as again can be seen from Eq. (B13).

5. SUMMARY

In our analysis we have ignored the residual helicity inner products $(\bar{u}_i\gamma^\mu u_i)$. From Eqs. (B11) and (B12) of Appendix B we see that these quantities become proportional to $(t)^{\frac{1}{2}}$ at large values of t. We now summarize our results for nondivergent graphs.

A. Nucleon–Meson Scattering

All planar nondivergent graphs have a leading behavior of $t^{\frac{1}{2}} \ln^{b-1} t$, where b is the maximum number of scaling sets compatible with delta function constraints and with compatible arrow configurations[1] that satisfy the following six conditions:

(i) They contain at least one t path.[1,2]

(ii) They have the property that no two external lines of the set are one and the same line.

(iii) They have the property that if l_i is any loop of the graph not belonging to the set then there is a partition[1] from loop l_i to either b_{12} or b_{34} not cutting any line of the scaling set.

(iv) They do not contain any line that when cut separates the set into two parts and at the same time does not belong to any t-path[1] lying entirely within the scaling set.

(v) The set contains only two external nucleon lines.

(vi) The set has the property that in traveling along that section of the open nucleon path lying in the set there can be only one occasion on which a $p_1(p_4)$ vertex of an m-line follows a $p_4(p_1)$ vertex of an m-line.

B. Nucleon–Nucleon Scattering

All planar nondivergent graphs have a leading behavior of $t^0 \ln^b t$, where b is the maximum number of scaling sets compatible with delta function constraints and with compatible arrow configurations, that satisfy the conditions (i)–(iv) and (vi) above and an amended fifth condition that

(v′) the set contains only four external nucleon lines.

C. Nucleon–Antinucleon Scattering

Planar nondivergent graphs have a leading behavior of $t^2 \ln^{b-1} t$, where b is the maximum number of scaling sets compatible with delta function constraints and with compatible arrow configurations that satisfy the first four conditions stated above together with the condition that

(v″) the set contains no external nucleon lines. If there does not exist such a set then the behavior is $t^1 \ln^{b-1} t$. The procedure for determining the leading behavior for divergent graphs is a simple generalization of the procedure stated in I.

ACKNOWLEDGMENTS

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APPENDIX A

Theorem: That part of the Feynman integral F_n for the n-rung ladder that has as numerator in I_G^1 the product $(p_1\cdot k_2)(k_2\cdot k_3)\cdots(k_i\cdot k_{i+1})\cdots(k_{n-1}\cdot p_4)$ does not contribute to the leading behavior of $t^0 \ln^{2n-3} t$.

Proof: We first prove the result for the three-rung ladder. We expand the integral

$$I_3 \equiv \int \prod_{i=1}^{2} d^4k_i \frac{(p_1\cdot k_2)(k_2\cdot p_4)}{\prod_{i=1}^{7}(Q_i^2 - m_i^2)}, \qquad \text{(A1)}$$

where Q_i is the momentum and m_i the mass of the ith line of the three-rung ladder, in a Chisholm series. In fact,

$$I_3 \propto \int \prod_{i=1}^{7} d\alpha_i\, \delta(\sum^{7} \alpha_i - 1) C^{-1}$$

$$\times [(-2)\, D^{-3}(p_1\cdot D_2)(p_4\cdot D_2) + D^{-2}\, D_{22}(p_1\cdot p_4)], \qquad \text{(A2)}$$

where

$$D_i^\mu = \frac{\partial D}{\partial b_i^\mu} \quad \text{and} \quad D_{ij} = \frac{1}{4}\frac{\partial^2 D}{\partial b_i^\mu\, \partial b_{j\mu}}.$$

Using the result of Tiktopoulos[2] we find the asymptotic behavior of I_3 is proportional to

$$t^0 \ln^3 t \int \prod (d\alpha) h^{-1}[(-)(-)\tfrac{1}{2}\cdot 4 + (-)2], \qquad \text{(A3)}$$

where $D \equiv gt + h$. The coefficient is zero and hence there is cancelation of leading behavior in the Chisholm series.

For the n-rung ladder, the coefficient of $t^0 \ln^{2n-3} t$ is proportional to

$$\sum_{i=1}^{n-1} A_i (i-1)!\,(-1)^{i-1},$$

where A_i is the number of terms in the $(n-i)$th term of the Chisholm series that gives the leading behavior. To prove that this sum is zero is a difficult combinatorial problem. We prove the result by the following method: $(p_4\cdot k_{n-1})$ can be written as $\frac{1}{2}(p_4 + k_{n-1})^2 - \frac{1}{2}m^2 - \frac{1}{2}k_{n-1}^2$, where $p_4^2 \equiv m^2$. With the first term we can cancel the propagator for line β_n, and the leading behavior for this part of the integral is t^0. The third term gives a leading behavior of $t^0 \ln^{2n-4} t$ since the scaling set β_n no longer generates a t^0 behavior.

Corollary 1: The result is true for the product

$$(p_1\cdot k_1)(k_1\cdot k_2)\cdots(k_{i-2}\cdot k_{i-1})(k_{i-1}\cdot k_{i+1}) \times (k_{i+1}\cdot k_{i+2})\cdots(k_{n-1}\cdot p_4).$$

We define an operator S_{α_j} such that

$$S_{\alpha_j}(q_1 k_{\alpha_j})(k_{\alpha_j}\cdot q_2) = (q_1\cdot q_2)k_{\alpha_j}^2.$$

Corollary 2: The term with numerator

$$S_{\alpha_1}\cdots S_{\alpha_M}(p_1 k_1)(k_1 k_2)\cdots (k_{i-2}\cdot k_{i-1})(k_{i-1}\cdot k_{i+1})(k_{i+1}\cdot k_{i+2})\cdots(k_{n-1}\cdot p_4)$$

does not contribute to the leading behavior unless $m = n - 2$.

Proof: If there exists an $\alpha_b = j$ then we can cancel the propagator $(k_j^2 - m_1^2)^{-1}$ of the nucleon line of loop l_j that is not a rung of the ladder. Thus we consider a ladder with m loops, each containing a contracted line. The analysis of the theorem is now directly applicable. Since the power of D in the basic term of the Chisholm series is $l + 1 - m$; the contraction of m lines, as far as D is concerned, is equivalent to reducing the number of loops by m. Further the coefficients are the same as for the graph where the m loops are omitted. The Corollary then follows.

There is, then, for order n, only $(n-1)$ terms in the original integrand that contribute to the leading behavior, corresponding to each of those nucleon lines, that are not rungs, being inactive.

APPENDIX B

I. The Calculation of $(\bar{u}_\alpha \gamma_i u_\beta)$

The calculation of the helicity inner products $(\bar{u}_\alpha \gamma_i u_\beta)$, where the suffixes α, β indicate both momentum and helicity variables is simply performed in the representation where γ_1, γ_2, γ_3 are skew-Hermitian and γ_4 is Hermitian. If $\mu_\alpha(\mathbf{p}_\alpha)$ is the helicity (three momentum) of the particle α and if we define the three vector $\mathbf{e}_\alpha \equiv (2\mu_\alpha)\mathbf{p}_\alpha\, |\mathbf{p}_\alpha|^{-1}$ then we can write

$$(\bar{u}_\alpha \gamma u_\beta) = \left[\frac{\mathbf{e}_\alpha + \mathbf{e}_\beta - i\mathbf{e}_\alpha \times \mathbf{e}_\beta}{1 + \mathbf{e}_\alpha\cdot\mathbf{e}_\beta}\right](\bar{u}_\alpha \beta\gamma_5 u_\beta) \qquad \text{(B1)}$$

$$(\bar{u}_\alpha \gamma_4 u_\beta) = \frac{1}{2m_1}(E_\alpha + m_1)^{\frac{1}{2}}(E_\beta + m_1)^{\frac{1}{2}} \times \left[1 + \frac{2\mu_\alpha\, |\mathbf{p}_\alpha|}{E_\alpha + m_1}\cdot\frac{2\mu_\beta\, |\mathbf{p}_\beta|}{E_\beta + m_1}\right] D^{\frac{1}{2}}_{\mu_\alpha\mu_\beta}(\alpha^{-1}\beta), \qquad \text{(B2)}$$

where $\beta = -\gamma_4$ and $D^{\frac{1}{2}}(\alpha^{-1}\beta)$ is the representation

in two-dimensional spinor space of the rotation matrix,

$$e^{-i\psi_\alpha J_3}\, e^{i\theta_\alpha J_2}\, e^{i(\psi_\alpha-\psi_\beta)J_3}\, e^{-i\theta_\beta J_2}\, e^{+i\psi_\beta J_3}, \tag{B3}$$

where θ_α, ψ_α are the polar angles of $\mathbf{p}_\alpha$ and $J_i (i = 1, 2, 3)$ are the three infinitesimal generators of the rotation group. Further,

$$(\bar{u}_\alpha \beta\gamma_5 u_\beta) = \frac{1}{2m_1}(E_\alpha + m_1)^{\frac{1}{2}}(E_\beta + m_1)^{\frac{1}{2}} \times \left[\frac{2\mu_\alpha\,|\mathbf{p}_\alpha|}{E_\alpha + m_1} + \frac{2\mu_\beta\,|\mathbf{p}_\beta|}{E_\beta + m_1}\right] D^{\frac{1}{2}}_{\mu_\alpha\mu_\beta}(\alpha^{-1}\beta). \tag{B4}$$

These are the results of Wichmann.[9]

II. The Calculation of $(\bar{u}_\alpha\gamma_i u_\beta^c)$

To calculate the helicity inner products $(\bar{u}_\alpha\gamma_i u_\beta^c)$, where the superscript c indicates the helicity spinor of the antinucleon, we follow the method of Wichmann.[9]

We use the relation

$$\Gamma_c^{-1} u^c_{\mu\beta} = (-i)2\mu_\beta u_{-\mu\beta},$$

where Γ_c is the matrix that transforms the γ-matrices into their complex conjugates—$\Gamma_c\gamma_i\Gamma_c^{-1} = \gamma_i^*$—to reduce the problem of calculating the inner products $(\bar{u}_\alpha\gamma u_\beta^c)$ to the problem already solved in the previous section of calculating the inner products $(\bar{u}_\alpha\gamma u_{-\beta})$.

In fact,

$$(\bar{u}_\alpha\gamma u_\beta^c) = (+i)2\mu_\beta \times \left[\frac{\mathbf{e}_\alpha - \mathbf{e}_\beta + i\mathbf{e}_\alpha\times\mathbf{e}_\beta}{1 - \mathbf{e}_\alpha\cdot\mathbf{e}_\beta}\right]\frac{1}{2m_1}(E_\alpha + m_1)^{\frac{1}{2}}(E_\beta + m_1)^{\frac{1}{2}} \times \left[1 - \frac{2\mu_\alpha\,|\mathbf{p}_\alpha|}{E_\alpha + m_1}\frac{2\mu_\beta\,|\mathbf{p}_\beta|}{E_\beta + m_1}\right] D^{\frac{1}{2}}_{\mu_\alpha-\mu_\beta}(\alpha^{-1}\beta) \tag{B5}$$

and

$$(\bar{u}_\alpha\gamma^4 u_\beta^c) = (+i)2\mu_\beta\frac{1}{2m_1}(E_\alpha + m_1)^{\frac{1}{2}}(E_\beta + m_1)^{\frac{1}{2}} \times \left[\frac{2\mu_\alpha\,|\mathbf{p}_\alpha|}{E_\alpha + m_1} - \frac{2\mu_\beta\,|\mathbf{p}_\beta|}{E_\beta + m_1}\right] D^{\frac{1}{2}}_{\mu_\alpha-\mu_\beta}(\alpha^{-1}\beta). \tag{B6}$$

III. High-Energy Limit of Inner Products

(a) Let us consider nucleon–nucleon scattering in the t channel with p_1, $p_2(p_3, p_4)$ the incoming (outgoing) momenta. Let us evaluate $(\bar{u}_4\gamma^\mu u_1)$ for the nucleon path (p_1, p_4) in the limit of large t and fixed s. In the center-of-mass system this limit demands that $\mathbf{p}_1 \sim \mathbf{p}_4$ since $\cos\theta \sim 1$. Expressions (B1), (B2) give in this limit

$$(\bar{u}_4\gamma u_1) \sim \frac{\mathbf{p}_1}{m_1}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \tag{B7}$$

$$(\bar{u}_4\gamma^4 u_1) \sim \frac{E_1}{m_1}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{B8}$$

Thus we derive the results of Federbush and Grisaru,

$$(\bar{u}_4\gamma^\alpha u_1) \sim (p_1^\alpha/m_1)\ \delta_{\mu_1\mu_4}. \tag{B9}$$

(b) Let us consider nucleon–nucleon scattering in the s channel with $p_1(p_4)$ an incoming (outgoing) nucleon momentum, then the limit of $(\bar{u}_4\cdot\gamma^\mu u_1)$ at large values of $t = (p_1 - p_4)^2$ is directly derivable from (B1)(B2). We find in the center-of-mass frame

$$(\bar{u}_4\gamma u_1) = \frac{|\mathbf{p}_1|}{m_1}\begin{pmatrix}(\cos\tfrac{1}{2}\theta\mathbf{i}_3 + \sin\tfrac{1}{2}\theta\mathbf{i}_-), & 0\\ 0, & -(\cos\tfrac{1}{2}\theta\mathbf{i}_3 + \sin\tfrac{1}{2}\theta\mathbf{i}_+)\end{pmatrix}, \tag{B10}$$

where $\mathbf{i}_i$ is the unit vector in the x_i direction and $\mathbf{i}_\pm = (\mathbf{i}_1 \pm i\mathbf{i}_2)$. As $\sin\tfrac{1}{2}\theta = (i/2\,|\mathbf{p}_1|)t^{\frac{1}{2}}$ and $\cos\tfrac{1}{2}\theta \sim (1/2\,|\mathbf{p}_1|)t^{\frac{1}{2}}$ becomes large,

$$(\bar{u}_4\gamma u_1) \sim \frac{1}{2m_1}\begin{pmatrix}(\mathbf{i}_3 + i\mathbf{i}_-), & 0\\ 0, & -(\mathbf{i}_3 + i\mathbf{i}_+)\end{pmatrix}t^{\frac{1}{2}} \tag{B11}$$

and,

$$(\bar{u}_4\gamma^4 u_1) \sim \frac{1}{2\,|\mathbf{p}_1|}\begin{pmatrix}E_1/m_1, & (-i)\\ (+i), & E_1/m_1\end{pmatrix}t^{\frac{1}{2}}. \tag{B12}$$

(c) Let us consider the limit at fixed s and large t for nucleon–antinucleon scattering in the s channel. In the center-of-mass frame the 3-momentum vectors $\mathbf{p}_3$, $\mathbf{p}_4$ of the final nucleon–antinucleon pair are antiparallel. Suppose $\mathbf{p}_4$ has coordinates $(\sin\theta, 0, \cos\theta)$. From (B5) and (B6) we find

$$(\bar{u}_4\gamma u_3^c) = (-i)\begin{pmatrix}(\mathbf{i}_3\cos\theta + \mathbf{i}_1\sin\theta), & (E_1/m_1)(\mathbf{i}_1\cos\theta - i\mathbf{i}_2 - \sin\theta\mathbf{i}_3)\\ (E_1/m_1)(\mathbf{i}_1\cos\theta + i\mathbf{i}_2 - \sin\theta\mathbf{i}_3), & -(\mathbf{i}_3\cos\theta + \mathbf{i}_1\sin\theta)\end{pmatrix} \tag{B13}$$

and

$$(\bar{u}_4\gamma^4 u_3^c) = \begin{pmatrix}0, & 0\\ 0, & 0\end{pmatrix}. \tag{B14}$$

[9] E. H. Wichmann (private communication).

Quasi-Classical Analysis of Coupled Oscillators

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A set of harmonic oscillators is coupled for a certain time, after which the coupling is removed. The initial and final states of the set are expressed as superpositions of the coherent states of the uncoupled oscillators, as in Glauber's formalism. It is shown that the expansion kernel for the final state can be obtained approximately by substituting into the kernel for the initial state the classical equations of motion of the amplitudes of the oscillators. The evolution of a density operator for the system can be similarly calculated. The approximation is the more exact, the longer the time of interaction compared with the periods of the uncoupled oscillators.

1. INTRODUCTION

THE electromagnetic fields in two adjacent cavities are initially in known quantum mechanical states, or in mixtures of states specified by given density operators. The fields are allowed to interact by opening an aperture between the cavities for an interval of time, after which the aperture is closed. The acts of opening and closing the aperture are assumed to induce no transitions in the fields. What are the final states of the fields in the cavities, and in particular, to what extent can they be calculated from the classical laws governing the electromagnetic field during the interaction?

These questions arise, for example, in studying the detection of signals received in the presence of thermal background radiation. One of the cavities represents an ideal receiver; the other is the outside world enclosed, for mathematical convenience, in a huge box. The receiver, initially empty, is exposed to the external field by opening an aperture for a certain time. After the aperture is closed, an observer is to decide by measuring the field in the receiver cavity whether a signal reached it during the exposure. It is necessary to find the density operators for the ultimate field in the receiver both in the presence and in the absence of a signal.

By means of an expansion in normal modes, the fields in the two cavities can be represented as an array of harmonic oscillators. While the aperture is open, these oscillators are coupled in a known way, and it is their temporal behavior under the coupling that is to be analyzed.

Alternatively, certain of the oscillators might represent modes of the electromagnetic field in a single cavity, the rest corresponding to modes of elastic vibration in the walls and providing a mechanism for dissipating energy from the electromagnetic field. How the interaction between the electromagnetic and the elastic oscillators causes a signal in the cavity to decay has been extensively studied.[1-3]

Feynman and Vernon have developed a method for treating such interacting systems by means of influence functionals.[4] They showed that the influence functional for a set of coupled harmonic oscillators is the exponential of a quadratic form depending on the mutual impedances among the oscillators as specified by classical electromagnetism. They suggested expanding the exponential function in a power series to obtain a perturbation analysis of the quantum mechanical behavior of the system. We wish to avoid such an expansion.

The Hamiltonian of a system of ν coupled harmonic oscillators is

$$H = \frac{1}{2}\sum_{k=1}^{\nu}\sum_{m=1}^{\nu}(T_{km}p_kp_m + V_{km}q_kq_m), \qquad (1.1)$$

where p_k and q_k are the momentum and coordinate operators of the kth oscillator, and T_{km} and V_{km} are certain known coefficients related to the kinetic and potential energies of the system. (With $\dot{q}_k = dq_k/dt$, the kinetic energy is

$$\frac{1}{2}\sum_{k=1}^{\nu}\sum_{m=1}^{\nu}R_{km}\dot{q}_k\dot{q}_m,$$

where the matrix $||R_{km}||$ is the inverse of the matrix $||T_{km}||$.) By a simple normalization the Hamiltonian can be written as

$$H = \tfrac{1}{2}\sum_k(p_k^2 + \omega_k^2q_k^2) + \tfrac{1}{2}\sum_{k\neq m}(T_{km}p_kp_m + V_{km}q_kq_m). \qquad (1.2)$$

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[1] I. R. Senitzky, Phys. Rev. 111, 3 (1958); 115, 227 (1959).
[2] J. Schwinger, J. Math. Phys. 2, 407 (1961).
[3] W. H. Louisell, *Radiation and Noise in Quantum Electronics* (McGraw-Hill Book Company, Inc., New York, 1964), pp. 255–259.
[4] R. P. Feyman and F. L. Vernon, Jr., Ann. Phys. (N. Y.) 24, 118 (1963).

It is helpful to think of the coupling among the oscillators as weak enough that for $k \neq m$,

$$|T_{km}| \ll 1, \qquad |V_{km}| \ll \min_n \omega_n^2,$$

although the main result of this paper requires only that the eigenfrequencies of the coupled system be of the same order of magnitude as those of the uncoupled system.

In the standard treatment of a set of coupled oscillators the Hamiltonian is reduced to a sum of squares,

$$H = \tfrac{1}{2} \sum_k (P_k^2 + \Omega_k^2 Q_k^2), \tag{1.3}$$

by introducing normal coordinates.[5,6] In the problems we are concerned with, however, the initial state of the system is expressed in terms of the states of the uncoupled set of oscillators, whose Hamiltonian is

$$H_0 = \tfrac{1}{2} \sum_k (p_k^2 + \omega_k^2 q_k^2), \tag{1.4}$$

and there is no simple relation between those states and the states of the normal modes. An analysis in terms of normal modes does not, apparently, lead to a connection between the initial and final states that can easily be related to the classical behavior of the system when those states refer to the uncoupled oscillators.

We introduce the creation and annihilation operators a_k^+ and a_k through the equations

$$\begin{aligned} q_k &= (\hbar/2\omega_k)^{\frac{1}{2}}(a_k^+ + a_k), \\ p_k &= i(\hbar\omega_k/2)^{\frac{1}{2}}(a_k^+ - a_k). \end{aligned} \tag{1.5}$$

They satisfy the commutation rules

$$\begin{aligned} a_k a_m^+ - a_m^+ a_k &= [a_k, a_m^+] = \delta_{km}, \\ [a_k, a_m] &= [a_k^+, a_m^+] = 0, \end{aligned} \tag{1.6}$$

and enable us to write the Hamiltonian as

$$H = H_0 + H_1 + H_2 \tag{1.7}$$

with H_0 the Hamiltonian of the uncoupled oscillators,

$$H_0 = (\tfrac{1}{2}\hbar) \sum_{k=1}^{r} \omega_k (a_k^+ a_k + a_k a_k^+), \tag{1.8}$$

and

$$\begin{aligned} H_1 &= (\tfrac{1}{2}\hbar) \sum_{k \neq m} D_{km}(a_k a_m^+ + a_k^+ a_m), \\ D_{km} &= (\omega_k \omega_m)^{\frac{1}{2}} T_{km} + (\omega_k \omega_m)^{-\frac{1}{2}} V_{km} = D_{mk}, \end{aligned} \tag{1.9}$$

$$\begin{aligned} H_2 &= (\tfrac{1}{2}\hbar) \sum_{k \neq m} E_{km}(a_k^+ a_m^+ + a_k a_m), \\ E_{km} &= (\omega_k \omega_m)^{-\frac{1}{2}} V_{km} - (\omega_k \omega_m)^{\frac{1}{2}} T_{km} = E_{mk}. \end{aligned} \tag{1.10}$$

We are especially concerned with the situation that the oscillators are initially uncoupled and in a known state or in a mixture of states described by a given density operator. The coupling is to be turned on, allowed to act for a time T, and then turned off; and the imposition and removal of the coupling are not to change the state of the system. We want to calculate the state of the system or its density operator after the coupling has been removed.

As explained by Louisell,[3] when the time dependence of the operator H_2 of Eq. (1.10) is examined, its terms are found to be proportional to $\exp[\pm i(\omega_k + \omega_m)t]$; and when the coupling acts for a time T containing many cycles of the oscillations of the system, these terms average out to nearly zero and have only a negligible effect on the system. The terms in H_1, on the other hand, have time dependences of the form $\exp[\pm i(\omega_k - \omega_m)t]$; and with ω_k and ω_m close together, they can be expected to have a long-term influence.

In this paper it is shown that the behavior of the system under the partial Hamiltonian $H' = H_0 + H_1$ can be treated to all orders of the coupling in terms of the classical laws of motion of the partial system. The remaining term H_2 can be included as a perturbation on this "quasi-classical" evolution, although this aspect of the problem is not extensively analyzed here.

The motion of the system under $H' = H_0 + H_1$ is worked out by means of Glauber's representations of the wavefunctions and density operators of the system in terms of coherent states of the simple harmonic oscillator.[7] The partial Hamiltonian can be written as

$$H' = (\tfrac{1}{2}\hbar) \sum_{k=1}^{r} \sum_{m=1}^{r} W_{km} a_k^+ a_m, \tag{1.11}$$

where $||W_{km}||$ is a Hermitian matrix, and this matrix is diagonalized by a unitary transformation of the operators a_k. The transformed operators and their associated coherent states have a simple time de-

[5] H. Goldstein, *Classical Mechanics* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1950), pp. 329–333.

[6] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill Book Company, Inc., New York, 1965).

[7] R. J. Glauber, Phys. Rev. **131**, 2766 (1963).

pendence, and the connection with the classical motion is easily established.

2. TRANSFORMATIONS OF COHERENT STATES

The state $|\Psi\rangle$ of the system can, at any fixed time t, be expressed in terms of the coherent states described by Glauber[7]:

$$|\Psi\rangle = \int |\alpha\rangle f(\alpha^+) \prod_k \left(\frac{d^2\alpha_k}{\pi}\right), \tag{2.1}$$

where α is a column vector of the complex numbers $\alpha_k, k = 1, 2, \cdots, \nu$, α^+ is the row vector $(\alpha_1^*, \cdots, \alpha_\nu^*)$, and $d^2\alpha_k = d\alpha_{kx}\, d\alpha_{ky}$ is an element of area in the complex α_k plane. The coherent state $|\alpha\rangle$ is the simultaneous right-eigenstate of the annihilation operators a_k, and it is generated from the vacuum state $|0\rangle$ by the displacement operators $D(\alpha_k)$,

$$|\alpha\rangle = \prod_k D(\alpha_k)\, |0\rangle, \tag{2.2}$$

the displacement operator $D(\alpha)$ being defined by

$$D(\alpha) = \exp(\alpha a^+ - \alpha^* a). \tag{2.3}$$

The function $f(\alpha^+)$ is related to $|\Psi\rangle$ by

$$f(\alpha^+) = \langle \alpha \mid \Psi\rangle. \tag{2.4}$$

[We have modified Glauber's notation by absorbing a factor $\exp(-\frac{1}{2}\alpha^+\alpha)$ into $f(\alpha^+)$ to shorten our expressions.] The representation in Eq. (2.1) is a consequence of the resolution of the identity

$$\mathbf{1} = \int |\alpha\rangle\langle\alpha| \prod_k \left(\frac{d^2\alpha_k}{\pi}\right) \tag{2.5}$$

and does not depend on our system's being composed of oscillators.

The representation of $|\Psi\rangle$ in Eq. (2.1) has a certain invariance under unitary transformations of the variables of the system. We define a new set $\mathbf{c}$ of annihilation operators c_m through the linear equations

$$\begin{aligned} c_m &= \sum_k U_{mk} a_k, \qquad c_m^+ = \sum_k U_{mk}^* a_k^+, \\ \mathbf{c} &= \mathbf{U}\mathbf{a}, \end{aligned} \tag{2.6}$$

where $\mathbf{a}$ denotes a column vector of the annihilation operators a_k and $\mathbf{U} = ||U_{mk}||$ is a unitary matrix,

$$\mathbf{U}\mathbf{U}^+ = \mathbf{U}^+\mathbf{U} = \mathbf{I} = ||\delta_{km}||. \tag{2.7}$$

The new operators c_k, c_k^+ obey the same commutation rules, Eq. (1.6), as the original ones a_k, a_k^+. In addition, if we define the complex amplitudes γ_m by

$$\gamma_m = \sum_k U_{mk}\alpha_k, \qquad \boldsymbol{\gamma} = \mathbf{U}\boldsymbol{\alpha}, \tag{2.8}$$

and observe that by Eq. (2.7), in the matrix notation to be used henceforth,

$$\begin{aligned} \mathbf{c}^+\boldsymbol{\gamma} - \boldsymbol{\gamma}^+\mathbf{c} &= \mathbf{a}^+\mathbf{U}^+\mathbf{U}\boldsymbol{\alpha} - \boldsymbol{\alpha}^+\mathbf{U}^+\mathbf{U}\mathbf{a} \\ &= \mathbf{a}^+\boldsymbol{\alpha} - \boldsymbol{\alpha}^+\mathbf{a}, \end{aligned} \tag{2.9}$$

we find by virtue of Eqs. (2.2) and (2.3) that

$$|\boldsymbol{\gamma}\rangle = \prod_m D(\gamma_m)\, |0\rangle = \prod_k D(\alpha_k)\, |0\rangle = |\boldsymbol{\alpha}\rangle, \tag{2.10}$$

and the states $|\boldsymbol{\alpha}\rangle$ and $|\boldsymbol{\gamma}\rangle$ are identical when the γ_m's and the α_k's determining them are related as in Eq. (2.8).

Returning now to Eq. (2.1) and bringing in the invariance of the volume element

$$\prod_m d^2\gamma_m = \prod_k d^2\alpha_k \tag{2.11}$$

under the unitary transformation of Eq. (2.8), we find that the state $|\Psi\rangle$ can as well be represented in the form

$$|\Psi\rangle = \int |\boldsymbol{\gamma}\rangle f'(\boldsymbol{\gamma}^+) \prod_m \left(\frac{d^2\gamma_m}{\pi}\right) \tag{2.12}$$

with

$$f'(\boldsymbol{\gamma}^+) = f[\boldsymbol{\alpha}^+(\boldsymbol{\gamma}^+)], \qquad \boldsymbol{\alpha}^+(\boldsymbol{\gamma}^+) = \boldsymbol{\gamma}^+\mathbf{U}. \tag{2.13}$$

The representation of an operator Q as[8]

$$\begin{aligned} Q &= \int |\boldsymbol{\alpha}\rangle \mathcal{Q}(\boldsymbol{\alpha}^+, \boldsymbol{\beta})\langle\boldsymbol{\beta}| \prod_k \left(\frac{d^2\alpha_k\, d^2\beta_k}{\pi^2}\right), \\ \mathcal{Q}(\boldsymbol{\alpha}^+, \boldsymbol{\beta}) &= \langle\boldsymbol{\alpha}|\, Q\, |\boldsymbol{\beta}\rangle \end{aligned} \tag{2.14}$$

possesses a similar invariance when the α_k's and the β_k's are transformed as in Eq. (2.8) into a new set of variables $\{\gamma_m\}$ and $\{\delta_m\}$,

$$\begin{aligned} \boldsymbol{\gamma} &= \mathbf{U}\boldsymbol{\alpha}, \qquad \boldsymbol{\delta} = \mathbf{U}\boldsymbol{\beta}, \\ \mathcal{Q}'(\boldsymbol{\gamma}^+, \boldsymbol{\delta}) &= \mathcal{Q}[\boldsymbol{\alpha}^+(\boldsymbol{\gamma}^+), \boldsymbol{\beta}(\boldsymbol{\delta})] = \mathcal{Q}(\boldsymbol{\gamma}^+\mathbf{U}, \mathbf{U}^+\boldsymbol{\delta}). \end{aligned} \tag{2.15}$$

3. TEMPORAL EVOLUTION OF THE SYSTEM

In particular, the unitary transformation matrix $\mathbf{U}$ can be taken as the one that diagonalizes the matrix $\mathbf{W} = ||W_{km}||$ in the partial Hamiltonian $H' = H_0 + H_1$,

$$\mathbf{W}' = ||\omega_k'\, \delta_{km}|| = \mathbf{U}\mathbf{W}\mathbf{U}^+. \tag{3.1}$$

Then if the state $|\Psi(0)\rangle$ of the system at time $t = 0$ is expressed in terms of a set of complex amplitudes $\boldsymbol{\alpha}_0$ through a function $f(\boldsymbol{\alpha}_0^+)$ as in Eq. (2.1), the state

[8] Reference 7, p. 2774.

at a later time t is, in the Schrödinger representation, approximately[9]

$$\begin{aligned}|\Psi(t)\rangle &\cong e^{-iH't/\hbar}\,|\Psi(0)\rangle \\ &= e^{-iH't/\hbar}\int |\boldsymbol{\alpha}_0\rangle f(\boldsymbol{\alpha}_0^+)\prod_k\left(\frac{d^2\alpha_{0k}}{\pi}\right) \\ &= \int e^{-iH't/\hbar}\,|\boldsymbol{\gamma}_0\rangle f'(\boldsymbol{\gamma}_0^+)\prod_m\left(\frac{d^2\gamma_{0m}}{\pi}\right) \\ &= \int |\exp(-i\mathbf{W}'t)\boldsymbol{\gamma}_0\rangle f'(\boldsymbol{\gamma}_0^+)\prod_m\left(\frac{d^2\gamma_{0m}}{\pi}\right), \\ f'(\boldsymbol{\gamma}_0^+) &= f(\boldsymbol{\gamma}_0^+\mathbf{U}).\end{aligned} \tag{3.2}$$

Here $\exp(-i\mathbf{W}'t)\boldsymbol{\gamma}_0$ is a column vector whose elements are $\gamma_{0m}\exp(-i\omega_m't)$, the matrix $\exp(-i\mathbf{W}'t)$ being diagonal with diagonal elements $\exp(-i\omega_m't)$. In Eq. (3.2) the γ_{0m}'s and the α_{0k}'s are related by the unitary transformation $\boldsymbol{\gamma}_0 = \mathbf{U}\boldsymbol{\alpha}_0$, as in Eq. (2.8). The approximation has been to neglect the term H_2 in the Hamiltonian.

Now, we use the inverse transformation $\mathbf{U}^+$ to define the complex amplitudes α_{tk} by

$$\begin{aligned}\boldsymbol{\alpha}_t &= \mathbf{U}^+\exp(-i\mathbf{W}'t)\boldsymbol{\gamma}_0 \\ &= \mathbf{U}^+\exp(-i\mathbf{W}'t)\mathbf{U}\boldsymbol{\alpha}_0 = \mathbf{V}(t)\boldsymbol{\alpha}_0, \\ \mathbf{V}(t) &= \mathbf{U}^+\exp(-i\mathbf{W}'t)\mathbf{U} = \exp(-i\mathbf{W}t),\end{aligned} \tag{3.3}$$

where the exponential function of a matrix is defined through its power-series expansion. The new transformation matrix $\mathbf{V}(t)$ is also unitary. By the same procedure as in Sec. 2, we equate the states $|\exp(-i\mathbf{W}'t)\boldsymbol{\gamma}_0\rangle$ with the states $|\boldsymbol{\alpha}_t\rangle$, and by using Eq. (2.13) we can write the state of the system at time t as

$$|\Psi(t)\rangle \cong \int |\boldsymbol{\alpha}_t\rangle f(\boldsymbol{\alpha}_0^+)\prod_k\left(\frac{d^2\alpha_{tk}}{\pi}\right), \tag{3.4}$$

in which the elements of $\boldsymbol{\alpha}_0^+$ are now linear functions of the elements α_{tk}^* of $\boldsymbol{\alpha}_t^+$ through the inverse of the unitary transformation in Eq. (3.3),

$$\boldsymbol{\alpha}_0 = \mathbf{V}^+(t)\boldsymbol{\alpha}_t, \qquad \boldsymbol{\alpha}_0^+ = \boldsymbol{\alpha}_0^+(\boldsymbol{\alpha}_t^+) = \boldsymbol{\alpha}_t^+\mathbf{V}(t). \tag{3.5}$$

The matrix $\mathbf{V}(t) = \exp(-i\mathbf{W}t)$ describes the classical behavior of a system of coupled oscillators whose Hamiltonian is $H' = H_0 + H_1$. If the complex amplitude of the mth oscillator at time t is taken as α_{tm}, it is related to the set $\{\alpha_{0k}\}$ of initial amplitudes by the same equations as in Eq. (3.3),

$$\alpha_{tm} = \sum_k V_{mk}(t)\alpha_{0k}.$$

This classical motion must be determined after eliminating the part of the interaction associated with the Hamiltonian H_2 of Eq. (1.10).

What we have shown is that if the state of the system is represented at time $t = 0$ by a superposition of coherent states $|\boldsymbol{\alpha}_0\rangle$ as in Eq. (2.1), the state at a later time t is given by a similar representation

$$\begin{aligned}|\Psi(t)\rangle &\cong \int |\boldsymbol{\alpha}_t\rangle f_t(\boldsymbol{\alpha}_t^+)\prod_k\left(\frac{d^2\alpha_{tk}}{\pi}\right), \\ f_t(\boldsymbol{\alpha}_t^+) &= f[\boldsymbol{\alpha}_0^+(\boldsymbol{\alpha}_t^+)] = f[\boldsymbol{\alpha}_t^+\mathbf{V}(t)],\end{aligned} \tag{3.6}$$

and the new representation function $f_t(\boldsymbol{\alpha}_t^+)$ is found by substituting into the original function $f(\boldsymbol{\alpha}_0^+)$ the relation in Eq. (3.5) between the initial set of amplitudes $\{\alpha_{0k}^*\}$ and the final set $\{\alpha_{tk}^*\}$.

If the system is not initially in a pure state, it must be described at time $t = 0$ by a density operator $\rho(0)$. This operator can be expressed in terms of the function[10]

$$R(\boldsymbol{\alpha}_0^+, \boldsymbol{\beta}_0) = \langle\boldsymbol{\alpha}_0|\,\rho(0)\,|\boldsymbol{\beta}_0\rangle \tag{3.7}$$

by an equation like Eq. (2.14). By the same reasoning as before, the density operator $\rho(t)$ at a later time t is given approximately by

$$\begin{aligned}\rho(t) &\cong e^{-iH't/\hbar}\rho(0)e^{iH't/\hbar} \\ &= \iint |\boldsymbol{\alpha}_t^+\rangle R_t(\boldsymbol{\alpha}_t^+, \boldsymbol{\beta}_t)\langle\boldsymbol{\beta}_t|\prod_k\left(\frac{d^2\alpha_{tk}\,d^2\beta_{tk}}{\pi^2}\right),\end{aligned} \tag{3.8}$$

in which the new expansion function is obtained from the original one of Eq. (3.7) by substituting for the elements of $\boldsymbol{\alpha}_0^+$ the expression in Eq. (3.5), and for the elements of $\boldsymbol{\beta}_0$ a similar one,

$$\begin{aligned}R_t(\boldsymbol{\alpha}_t^+, \boldsymbol{\beta}_t) &= R[\boldsymbol{\alpha}_0^+(\boldsymbol{\alpha}_t^+), \boldsymbol{\beta}_0(\boldsymbol{\beta}_t)] \\ &= R[\boldsymbol{\alpha}_t^+\mathbf{V}(t), \mathbf{V}^+(t)\boldsymbol{\beta}_t].\end{aligned} \tag{3.9}$$

The function $R_t(\boldsymbol{\alpha}_t^+, \boldsymbol{\beta}_t)\exp\frac{1}{2}(\boldsymbol{\alpha}_t^+\boldsymbol{\alpha}_t + \boldsymbol{\beta}_t^+\boldsymbol{\beta}_t)$ is the generating function of the matrix elements of the density operator $\rho(t)$ in the number representation.[10]

If, in particular, the system can be described at time $t = 0$ by a density function $P(\boldsymbol{\alpha})$,[11]

$$\rho(0) = \int P(\boldsymbol{\alpha}_0)\,|\boldsymbol{\alpha}_0\rangle\langle\boldsymbol{\alpha}_0|\prod_k(d^2\alpha_{0k}), \tag{3.10}$$

it is described at a later time t by the density function $P_t(\boldsymbol{\alpha}_t)$ obtained, with the same neglect of H_2, by substituting from Eq. (3.5) into $P(\boldsymbol{\alpha}_0)$:

$$P_t(\boldsymbol{\alpha}_t) = P[\mathbf{V}^+(t)\boldsymbol{\alpha}_t], \tag{3.11}$$

and the density operator at the later time t is approximately

[9] Reference 7, p. 2771.

[10] Reference 7, p. 2775.

[11] Reference 7, p. 2776.

$$\rho(t) \cong \int P_t(\alpha_t)\ |\alpha_t\rangle\langle\alpha_t|\ \prod_k (d^2\alpha_{tk}). \tag{3.12}$$

In all these expressions the quantities α_{tk}, β_{tk}, and so on, are merely variables of integration, and the subscripts t can be dropped once all the substitutions have been made.

4. EFFECT OF THE REMAINDER H_2

The effect of neglecting the term H_2 of the Hamiltonian can now be assessed more precisely. We transform it by substituting for the a_k's in Eq. (1.10) the c_k's defined by Eq. (2.6), with the unitary matrix $\mathbf{U}$ taken as the one that reduces the partial Hamiltonian H' to diagonal form

$$H' = (\tfrac{1}{2}\hbar) \sum_k \omega'_k(c_k c_k^+ + c_k^+ c_k). \tag{4.1}$$

Then H_2 becomes

$$\begin{aligned} H_2 &= (\tfrac{1}{2}\hbar) \sum_{k\neq m} (E'^*_{km} c_k^+ c_m^+ + E'_{km} c_k c_m), \\ E'_{km} &= \sum_i \sum_n E_{in} U^*_{ki} U^*_{mn}. \end{aligned} \tag{4.2}$$

If we transform to the interaction representation in which the states are the Schrödinger states of the Hamiltonian $H' = H_0 + H_1$, the effect of the term H_2 is embodied in the unitary operator[12]

$$\Upsilon_2(t) = \exp\left[-i \int_0^t H_2(t')\, dt'/\hbar\right] \tag{4.3}$$

which operates on those states. Here

$$\begin{aligned} H_2(t) &= e^{+iH't/\hbar} H_2 e^{-iH't/\hbar} \\ &= (\tfrac{1}{2}\hbar) \sum_{k\neq m} \{E'^*_{km} c_k^+ c_m^+ \exp[i(\omega'_k + \omega'_m)t] \\ &\qquad + E'_{km} c_k c_m \exp[-i(\omega'_k + \omega'_m)t]\}, \end{aligned} \tag{4.4}$$

where $\omega'_k/2\pi$ are the eigenfrequencies of the partial Hamiltonian H'. We suppose that the coupling is weak enough that the eigenfrequencies $\omega'_k/2\pi$ are of the same order of magnitude as the frequencies $\omega_k/2\pi$ of the uncoupled system.

A perturbation expansion of the operator $\Upsilon_2(t)$ leads to

$$\begin{aligned} \Upsilon_2(t) &= \mathbf{1} - i \int_0^t \frac{H_2(t')\, dt'}{\hbar} + \cdots \\ &= \mathbf{1} - \tfrac{1}{2} \sum_{k\neq m} (E'^*_{km} c_k^+ c_m^+ (\omega'_k + \omega'_m)^{-1} \\ &\quad \times \{\exp[i(\omega'_k + \omega'_m)t] - 1\} \\ &\quad + E'_{km} c_k c_m (\omega'_k + \omega'_m)^{-1} \\ &\quad \times \{1 - \exp[-i(\omega'_k + \omega'_m)t]\}) + \cdots \end{aligned} \tag{4.5}$$

and the factors $(\omega'_k + \omega'_m)^{-1}$ in these and succeeding terms make $\Upsilon_2(t) - \mathbf{1}$, $t \geq T$, negligible whenever the time T of interaction is much greater than the longest period of any of the oscillations.

5. APPLICATIONS

Suppose that the oscillators represent the modes of the electromagnetic field of a cavity. If the cavity contains at time $t = 0$ a coherent field superposed on the thermal radiation, the initial density operator $\rho(0)$ can be expressed as in Eq. (3.10) in terms of a density function of the form[13]

$$\begin{aligned} P(\alpha_0) &= \pi^{-\nu} |\det \varphi_0|^{-1} \\ &\quad \times \exp[-(\alpha_0^+ - \mathfrak{y}_0^+)\varphi_0^{-1}(\alpha_0 - \mathfrak{y}_0)], \end{aligned} \tag{5.1}$$

where ν is the number of significant modes and $\mathfrak{y}_0$ is a column vector of the mode amplitudes μ_{k0} of the coherent part of the field at $t = 0$. (If the thermal radiation were absent, the field would be in the coherent state $|\mathfrak{y}_0\rangle$.) The elements of the mode correlation matrix φ_0 are

$$(\varphi_0)_{km} = \mathrm{Tr}\,[\rho(0) a_m^+ a_k] - \mu^*_{0m}\mu_{0k}. \tag{5.2}$$

When the matrix φ_0 is diagonal, its diagonal elements are the mean numbers of photons in the modes of the field due to the thermal radiation, and those mean numbers are given by the Planck's law.

The density operator $\rho(t)$ at a later time t is given in our approximation by Eq. (3.12), with the density function

$$\begin{aligned} P_t(\alpha_t) &= \pi^{-\nu} |\det \varphi_0|^{-1} \\ &\quad \times \exp[-(\alpha_t^+ \mathbf{V} - \mathfrak{y}_0^+)\varphi_0^{-1}(\mathbf{V}^+\alpha_t - \mathfrak{y}_0)], \\ \mathbf{V} &= \mathbf{V}(t), \end{aligned} \tag{5.3}$$

according to Eq. (3.11). Defining the mode correlation matrix at time t by

$$\varphi_t = \mathbf{V}(t)\varphi_0\mathbf{V}^+(t), \tag{5.4}$$

and the vector of coherent field amplitudes at time t by

$$\mathfrak{y}_t = \mathbf{V}(t)\mathfrak{y}_0, \tag{5.5}$$

we see that the density function at time t is also of the Gaussian form,

$$\begin{aligned} P_t(\alpha_t) &= \pi^{-\nu} |\det \varphi_t|^{-1} \\ &\quad \times \exp[-(\alpha_t^+ - \mathfrak{y}_t^+)\varphi_t^{-1}(\alpha_t - \mathfrak{y}_t)]. \end{aligned} \tag{5.6}$$

Hence in this approximation a Gaussian density function remains Gaussian with the passage of time.

[12] Reference 3, p. 61.

[13] Reference 7, p. 2786.

It may be that at time t we are able to make measurements on only a subset of the oscillators. In the case of two cavities coupled through an aperture, mentioned in the Introduction, it may be only the field in the one cavity, corresponding to the receiver, that can be observed. Similarly, for the cavity whose field is coupled to a set of elastic modes providing a loss mechanism, only the oscillators representing the electromagnetic field are accessible. We then need only a density operator $\rho'(t)$ for the observable subset of oscillators, and this can be obtained by taking the trace of $\rho(t)$ over the states of the unobserved oscillators.

This trace is carried out in Glauber's representation, Eq. (3.12), by integrating the density function $P_t(\boldsymbol{\alpha}_t)$ over the α_{tk}'s corresponding to the unobserved part of the system. When this density function is Gaussian, as in Eq. (5.6), the integrations result in a new density function that is also Gaussian and of the same form as before. The new correlation matrix $\boldsymbol{\varphi}_t'$ is obtained from the original one $\boldsymbol{\varphi}_t$ by striking out the rows and columns referring to the unobserved oscillators. Since the matrix $\mathbf{V} = \mathbf{V}(t)$ can be obtained from the classical laws of motion of the set of oscillators, the new density function can be written down in this quasi-classical approximation once the problem of the classical behavior of the system has been solved.

When there are only two oscillators, 1 and 2, involving before the interaction the annihilation operators a_{01}, a_{02} and afterward the annihilation operators a_{t1}, a_{t2}, the unitary transformation connecting these as in Eq. (3.3) has the simple form

$$\begin{aligned} a_{t1} &= \lambda a_{01} + \lambda' a_{02}, \\ a_{t2} &= \lambda' a_{01} + \lambda^* a_{02}, \\ \lambda' &= [1 - |\lambda|^2]^{\frac{1}{2}}. \end{aligned} \tag{5.7}$$

Takahasi[14] has shown how to obtain the final density operator $\rho(t)$ for such a system from an initial one $\rho(0)$ by taking the coordinate operators q_{01}, q_{02}, q_{t1}, q_{t2} also to be related as in Eq. (5.7) and expanding an initial Schrödinger wavefunction in the coordinate representation as a series of Schrödinger wavefunctions in q_{t1},q_{t2}. These wavefunctions are products of Hermite functions. He presented detailed results for a system in which one of the oscillators is initially in a mixture of states characteristic of Gaussian thermal noise, and he averaged over the states of this oscillator to obtain the final density operator for the other oscillator alone. Takahasi's results can be obtained quite directly by means of Eq. (3.9).

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[14] H. Takahasi, in *Advances in Communication Systems*, A. Balakrishnan, Ed. (Academic Press Inc., New York, 1965), Vol. 1, p. 227.

Calculation of Exchange Second Virial Coefficient of a Hard-Sphere Gas by Path Integrals*

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By direct examination of the path (Wiener)-integral representation of the diffusion Green's function in the presence of an opaque sphere, we are able to obtain upper and lower bounds for that Green's function. These bounds are asymptotically correct for short-time, even in the shadow region. Essentially, we have succeeded in showing that diffusion probabilities for short-time intervals are concentrated mainly on the optical path. By integrating the Green's function, we obtain upper- and lower-bound estimates for the exchange part of the second virial coefficient of a hard-sphere gas. We can show that, for high temperature, it is asymptotically very small compared to the corresponding quantity for an ideal gas, viz.,

$$B_{exch}/B^0_{exch} = \exp\{-\tfrac{1}{2}\pi^3(a/\Lambda)^2 + O[(a/\Lambda)^{2/3}]\},$$

where Λ is the thermal wavelength and a is the hard-sphere radius. While it was known before that B_{exch}/B^0_{exch} is exponentially small for high temperatures, this is the first time that a precise asymptotic formula is both proposed and proved to be correct.

I. INTRODUCTION

FOR a gas of particles that interact via a two-body potential, the calculation of the second virial coefficient[1] involves an analysis of only a two-body problem. This simplification holds for quantum as well as for classical mechanics, but there the similarity between the two kinds of mechanics ends. Classically, the second virial coefficient depends neither on particle mass, m, nor on statistics and, for a one-component gas, is given by the simple configuration integral:

$$B_{cl}(T) = \tfrac{1}{2}N\int d\mathbf{r}\{1 - \exp[-\beta v(\mathbf{r})]\}, \qquad (1.1)$$

where $v(\mathbf{r})$ is the pair potential, N is Avogadro's number, and $\beta = (kT)^{-1}$.

Quantum-mechanically, no such simple formula as (1.1) exists, for the calculation of $B(T)$ requires either a detailed knowledge of the solutions of the two-particle Schrödinger equation at all energies, or, alternatively, a solution of the corresponding diffusion problem. Thus, while the problem of calculating the second virial coefficient may not be as profound as the original many-body problem from which it arose, it does require the answer to interesting questions about the classical analysis of the three-dimensional diffusion equation. To become familiar with the problem is to realize how difficult it is to calculate quantum corrections to (1.1).[2]

The true physicist will doubtless inquire whether quantum corrections to (1.1) are in fact significant, and the answer is that for helium they are quite important. Even for temperatures as high as 60°K, the quantum corrections in helium are about a third of the total.[3] For a hard-sphere gas, the quantum corrections do not drop to a tenth of the total until a temperature of about 1200°K is reached.[4] Since experimental values of the second virial coefficient are used in attempting to determine the effective inter-atomic helium potential, these quantum corrections are certainly worthy of consideration.

There is also[3] a pronounced difference between the second virial coefficient of He^3 and He^4, especially below 60°K. Assuming (as is always done) that the interaction potential is the same for the two isotopes, the difference could conceivably come from three sources: (a) the atomic mass difference; (b) the difference in nuclear spin which affects the statistical weights; and (c) the difference between Fermi–Dirac and Bose–Einstein statistics. For an ideal (noninteracting) quantum gas (b) and (c) are everything [see Eq. (1.11) below], and one might be tempted to conclude that, for helium too, the isotopic mass difference was relatively unimportant. Numerical calculations have, however, indicated the

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[1] The nth-virial coefficient is the temperature-dependent coefficient of v^{-n+1} in the series

$$Pv = RT[1 + B(T)v^{-1} + C(T)v^{-2} + \cdots].$$

Here, P is the pressure, T is the temperature, R is the gas constant, and v is the volume per mole of gas. In terms of N (Avogadro's number), $v = N\rho^{-1}$ and $R = Nk$, where ρ is the particle number density and k is Boltzmann's constant.

[2] Hugh E. DeWitt, J. Math. Phys. **3**, 1003 (1962).

[3] J. Kilpatrick, W. Keller, E. Hammel, and N. Metropolis, Phys. Rev. **94**, 1103 (1954); J. Kilpatrick, W. Keller, and E. Hammel, *ibid.* **97**, 9 (1955).

[4] F. Mohling, Phys. Fluids **6**, 1097 (1963).

reverse. Above about 4°K, almost all of the difference in the two second virial coefficients is a mass effect.[3] This difference is about 10% at 60°K and drops only to the order of 5% at room temperature. In other words, on the one hand the mass effect is unusually large for helium, while on the other hand the effects due to statistics and spin decrease very rapidly with increasing temperature. For an ideal gas, these latter effects decrease as $T^{-\frac{3}{2}}$, but for helium the decrease is far more rapid. Under the assumption that the repulsive part of the helium interaction potential can be effectively replaced by a hard core, it has been *proved*[5] that the statistical and spin effects decrease *at least* exponentially fast with increasing temperature (for high temperatures). The suppression of exchange effects is so rapid that 20°K may be considered to be a high temperature for which asymptotic formulas are reasonably valid.

It is the purpose of this paper to prove that the exponential law for the hard-sphere gas mentioned above is more than just an upper bound, that it is in fact correct. The true coefficient appearing in the law [cf., (1.13) below] is, however, different from that of the bound given in Ref. 5, although the correct value was stated there, without proof, in a footnote.

To the casual reader, the problem must seem almost trivial. In the first place, we have eschewed calculating the true equation of state, and have, instead, contented ourselves with examining only the second virial coefficient—a simple matter of a two-body problem. Secondly, we are examining only the effects of spin and statistics. Thirdly, we are confining ourselves to high temperatures. That there is no simple perturbation theory for this problem must appear strange. But it is a fact that, in many respects, the problem is similar to the classical problem of diffraction of waves (of short wavelength) around a sphere into the dark zone, a problem which has exercised mathematicians for years.

The mathematical statement of the problem is as follows: The quantum-mechanical second virial coefficient may be written as the sum of a direct and an exchange part,

$$B = B_{\text{direct}} + B_{\text{exch}}, \tag{1.2}$$

where

$$B_{\text{direct}} = \tfrac{1}{2}N \int d\mathbf{r}\, [1 - 2^{\frac{3}{2}}\Lambda^3 G(\mathbf{r}, \mathbf{r}; \beta)], \tag{1.3}$$

$$B_{\text{exch}} = \mp\sqrt{2}\, \Lambda^3 N(2S+1)^{-1} \int d\mathbf{r}\, G(\mathbf{r}, -\mathbf{r}; \beta), \tag{1.4}$$

and

$$\Lambda^2 = 2\pi\hbar^2\beta/m. \tag{1.5}$$

In (1.4) the $-$ sign is for bosons and the $+$ sign is for fermions. S is the total spin of the atom (the nuclear spin alone in the case of helium), it is to be noted that the spin enters only into B_{exch}. Thus, (b) and (c) mentioned above go together.

The function $G(\mathbf{r}, \mathbf{r}'; t)$ is the diffusion Green's function (also known as the Bloch function), and it satisfies

$$[-D\nabla_{\mathbf{r}}^2 + v(\mathbf{r}) + \partial/\partial t]G(\mathbf{r}, \mathbf{r}', t) = 0, \quad (\text{for } t > 0) \tag{1.6}$$

with the initial condition

$$\lim_{t\to 0} G(\mathbf{r}, \mathbf{r}'; t) = \delta(\mathbf{r} - \mathbf{r}'). \tag{1.7}$$

In addition, G satisfies appropriate boundary conditions in $\mathbf{r}$, such as vanishing on the walls of a box. In our case, we are interested in the limit of an infinite volume which means that G satisfies (1.6) for all $\mathbf{r}$ but vanishes when $r \to \infty$. It is to be noted that boundary conditions need only be defined with respect to $\mathbf{r}$. Despite this fact, and despite the fact that (1.6) refers really only to $\mathbf{r}$, G automatically turns out to be a symmetric function of $\mathbf{r}$ and $\mathbf{r}'$ for all t.

Equation (1.6) describes diffusion in a potential $v(\mathbf{r})$, with $\mathbf{r}'$ the source point, t the elapsed time, and D the diffusion constant. For quantum-mechanical purposes, t is interpreted as β, v is the interparticle potential, and D is related to the mass of a single atom by

$$D = \hbar^2/m \equiv \tfrac{1}{4}\alpha. \tag{1.8}$$

Thus,

$$\Lambda^2 = 2\pi\, Dt = \tfrac{1}{2}\pi\alpha t. \tag{1.9}$$

In the case of *no interaction* ($v = 0$), G is given by

$$G_0(\mathbf{r}, \mathbf{r}', t) = (\pi\alpha t)^{-\frac{3}{2}} \exp[-(\mathbf{r} - \mathbf{r}')^2/\alpha t], \tag{1.10}$$

and when this is inserted into (1.3) and (1.4), we obtain the result:

$$B^0_{\text{direct}} = 0, \tag{1.11a}$$

$$B^0_{\text{exch}} = \mp N\Lambda^3 2^{-5/2}(2S+1)^{-1}. \tag{1.11b}$$

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[5] S. Larsen, J. Kilpatrick, E. Lieb, and H. Jordan, Phys. Rev. **140**, A129 (1965). While it was realized in Ref. 4 that exchange effects are small at high temperatures, no proof of this assertion nor statement of its exponential character were offered. For further results on the hard sphere problem, see the following papers: M. Boyd, S. Larsen, and J. Kilpatrick, J. Chem. Phys. **45**, 499 (1966); S. Larsen, K. Witte, and J. Kilpatrick, J. Chem. Phys. (to be published). Recently, J. B. Keller and R. A. Handelsman, Phys. Rev. **148**, 94 (1966), have calculated the first few terms in a high-temperature power series for the *direct* second virial coefficient of a hard-sphere gas.

For a hard-sphere potential,

$$v(r) = \infty, \quad \text{for} \quad r \leq a, \qquad = 0, \quad \text{for} \quad r > a, \tag{1.12}$$

Eq. (1.11b) is a very misleading approximation to B_{exch} for high temperatures. We are to *prove* that, for small t or Λ,

$$\ln \left\{ \frac{B_{\text{exch}}}{B^0_{\text{exch}}} \right\} = -\frac{\pi^3}{2} \left(\frac{a}{\Lambda} \right)^2 + O\left(\left(\frac{a}{\Lambda} \right)^{\frac{5}{2}} \right). \tag{1.13}$$

The proof consists in obtaining upper and lower bounds for $G(\mathbf{r}, \mathbf{r}'; t)$ by means of Wiener, or path integrals. These bounds are valid for all temperatures, and we could, in fact, give a more detailed estimate than is indicated in (1.13). The bounds are, however, complicated functions of t, and it seems neither necessary nor desirable to go beyond the asymptotic formula in (1.13).

Before giving the proof, it is worthwhile mentioning an alternative formulation of the problem which, at first sight, seems to offer an immediate solution. For a particle in a box, we can write

$$G(\mathbf{r}, \mathbf{r}'; t) = \sum_{n=1}^{\infty} \exp(-te_n) \psi_n(\mathbf{r}) \psi_n^*(\mathbf{r}'), \tag{1.14}$$

where e_n is the nth energy level and ψ_n is the corresponding normalized eigenfunction. When (1.14) is inserted into (1.3) and (1.4), it is seen that knowledge of the energy levels alone is required. When the box is very large compared to the range of the potential, the virial coefficient can be expressed in terms of the bound-state energy levels (if any) and the scattering phase shifts of the potential, viz.

$$B_{\text{direct}} = -\sqrt{2}\, N\Lambda^3 \sum_{\text{all } l} (2l+1) B_l, \tag{1.15a}$$

$$B_{\text{exch}} = B^0_{\text{exch}} \mp (2S+1)^{-1} \sqrt{2}\, N\Lambda^3 \times \{ \sum_{l \text{ even}} - \sum_{l \text{ odd}} \} (2l+1) B_l, \tag{1.15b}$$

where

$$B_l = \sum_n \exp[-\beta e_n(l)] + (\Lambda^2/\pi^2) \int_0^\infty e^{-\Lambda^2 k^2/2\pi} \eta_l(k) k\, dk. \tag{1.16}$$

In (1.16) the sum is over negative energy levels (if any), while the integral contains the phase shift η_l—all for the appropriate angular momentum, l. For the case of no bound state, the above formula for the second virial coefficient in terms of the phase shifts was apparently first stated by Gropper and by Beth and Uhlenbeck,[6] and a derivation of it can be found in Ref. 3.

For the hard-sphere potential, there are no bound states, and it would appear that (1.16) and (1.15) should give the answer simply, especially as the phase shifts are given by the elementary formula

$$\eta_l(k) = -\tan^{-1} \{ (-1)^l J_{l+\frac{1}{2}}(ka) / J_{-l-\frac{1}{2}}(ka) \}. \tag{1.17}$$

For small Λ, however, we see that large values of k are important in (1.16). For very large k, the sum on l in (1.15b) may be performed with the aid of Watson's transformation, and it is similar to the problem of diffraction around a sphere at short wavelength.[7] Apart from certain technical convergence difficulties connected with the fact that we are really interested in the diffracted field on a diameter (that is to say a caustic), there is another more important problem.[8] This problem is that there may also be contributions to (1.16) from small k, a region where Watson's transformation is not of great use. Finite k contributions would, from (1.16), be expected to give a power series in Λ for small Λ. But it is a fact that there is a remarkable cancellation between even and odd l in (1.15b) so that *every* term in this power series vanishes. The final result, as shown in (1.13), is a function that vanishes faster than any power as $\Lambda \to 0$. If the potential were finite, instead of a hard core, this power series would *not* vanish. Thus, in summary, (1.16) and (1.15b) is a difficult starting point for hard spheres, despite the simplicity of the phase shifts and the existence of Watson's transformation.

Our approach is to go back to (1.4) and, as we mentioned before, to estimate $G(\mathbf{r}, -\mathbf{r}; t)$ directly through its expression in terms of a Wiener integral. Such integrals play an important theoretical role in analysis but, unless the integrand is Gaussian, it is difficult to obtain numerical answers from them. There have, of course, been rare exceptions such as Feynman's treatment of the Polaron problem.[9] Nevertheless, the analysis presented here is one of the very few cases, if not the only one, in which both an upper *and* a lower bound to a function is obtained with path integrals. The path integral approach also has the great virtue of transparency because it brings out the close connection between the diffusion equation, (1.6), and a random walk

[6] L. Gropper, Phys. Rev. **51**, 1108 (1937); E. Beth and G. Uhlenbeck, Physica **4**, 915 (1937); see also G. Uhlenbeck and E. Beth, *ibid.* **3**, 729 (1936).

[7] B. Levy and J. Keller, Commun. Pure Appl. Math. **12**, 159 (1959), where the relevent asymptotic formulas are given on p. 201. See also J. Keller, J. Opt. Soc. Am. **52**, 116 (1962).

[8] I am indebted to Dr. S. Larsen for pointing this out to me.

[9] R. Feynman, Phys. Rev. **97**, 660 (1955).

problem. For these reasons, we believe the sequel might also possess an intrinsic mathematical value.

II. LOWER BOUND BY PATH INTEGRALS

The solution to (1.6) and (1.7) is easily shown to be unique and to satisfy the relation

$$G(\mathbf{r}, \mathbf{r}'; t) = \int d\mathbf{z}\, G(\mathbf{r}, \mathbf{z}; t_1) G(\mathbf{z}, \mathbf{r}'; t_2) \qquad (2.1)$$

for any positive t_1 and t_2 such that $t_1 + t_2 = t$. If the time interval t is divided into $n + 1$ intervals of duration Δ, so that $t = (n + 1)\Delta$, then, from (2.1),

$$\begin{aligned} G(\mathbf{r}, \mathbf{r}'; t) &= \lim_{n\to\infty} \int d\mathbf{Z}\, G(\mathbf{r}, \mathbf{z}_1; \Delta) G(\mathbf{z}_1, \mathbf{z}_2; \Delta) \cdots \\ &\quad \times G(\mathbf{z}_{n-1}, \mathbf{z}_n; \Delta) G(\mathbf{z}_n, \mathbf{r}', \Delta) \\ &= \lim_{n\to\infty} \int d\mathbf{Z}\, G_0(\mathbf{r}, \mathbf{z}_1; \Delta) e^{-\Delta v(\mathbf{z}_1)} \\ &\quad \times G_0(\mathbf{z}_1, \mathbf{z}_2; \Delta) e^{-\Delta v(\mathbf{z}_2)} \cdots \\ &\quad \times e^{-\Delta v(\mathbf{z}_{n-1})} G_0(\mathbf{z}_{n-1}, \mathbf{z}_n; \Delta) \\ &\quad \times e^{-\Delta v(\mathbf{z}_n)} G_0(\mathbf{z}_n, \mathbf{r}'; \Delta), \end{aligned} \qquad (2.2)$$

where $d\mathbf{Z} = d\mathbf{z}_1\, d\mathbf{z}_2 \cdots d\mathbf{z}_n$.

The heuristic justification for (2.2) is that, if $\alpha = 4D$ were zero, then

$$G(\mathbf{r}, \mathbf{r}'; \Delta) = \delta(\mathbf{r} - \mathbf{r}') \exp[-\Delta v(\mathbf{r})],$$

whereas if $v = 0$ then $G = G_0$, which is very nearly $\delta(\mathbf{r} - \mathbf{r}')$ for small Δ. The combination

$$G_0(\mathbf{r}, \mathbf{r}'; \Delta) \exp[-\Delta v(\mathbf{r})]$$

is, hopefully, a good approximation to G [at least as far as the integral in (2.2) is concerned] for very small Δ. Formally, this combination satisfies (1.6) to leading order in Δ *for those values of* $\mathbf{r}$ *and* $\mathbf{r}'$ *such that* $G(\mathbf{r}, \mathbf{r}'; \Delta)$ *significantly contributes to* (2.2).

The fact that (2.2) is correct for a large class of bounded potentials has been known for some time. We are interested, however, in the hard-core potential [see Eq. (2.3) below] for which a special proof is apparently required. We remark that Ginibre has previously used (2.2) for the hard-core case, but without giving an explicit proof.[10]

I am indebted to Professor D. Babbitt for the proof in the hard-core case, which is outlined as the following. Take $D = \frac{1}{4}$ for convenience, and let Ω be the set of functions (paths) from $[0, \infty)$ into $\dot{\mathfrak{R}}^3$, where $\dot{\mathfrak{R}}^3$ is the one-point compactification of $\mathfrak{R}^3$, the three-dimensional Euclidean space. Let $\{P_{\mathbf{r},\mathbf{r}';t};\ \mathbf{r}, \mathbf{r}' \in \mathfrak{R}^3,\ t > 0\}$ denote the family of conditional Wiener measures on Ω as defined by Ginibre.[11] The crucial point to note is that $P_{\mathbf{r},\mathbf{r}';t}$ is concentrated on the paths that are bounded and continuous on $[0, t]$. Denote integration of $P_{\mathbf{r},\mathbf{r}';t}$ integrable functionals, F, on Ω, by $\int F(\omega) P_{\mathbf{r},\mathbf{r}';t}(d\omega)$, where ω denotes a generic path in Ω. Let

$$\Omega_t(\omega) = \begin{cases} 1 & \text{if } |\omega(\tau)| > a \text{ for all } 0 < \tau \leq t, \\ 0 & \text{otherwise.} \end{cases}$$

Then Ω_t is $P_{\mathbf{r},\mathbf{r}';t}$ integrable and

$$G(\mathbf{r}, \mathbf{r}'; t) = \int \Omega_t(\omega) P_{\mathbf{r},\mathbf{r}';t}(d\omega).$$

This result is essentially given, with different notation, by Ray.[12] Since $P_{\mathbf{r},\mathbf{r}';t}$ is concentrated on the bounded, continuous paths on $[0, t]$, it follows that

$$\lim_{n\to\infty} \left\{ \prod_{k=1}^{n} \theta\left[\omega\left(\frac{kt}{n+1} \right) \right] \right\} = \Omega_t(\omega)$$

$P_{\mathbf{r},\mathbf{r}';t}$—almost everywhere on Ω. The function θ is defined in Eq. (2.3) below. Hence, applying the dominated convergence theorem we have

$$\begin{aligned} \lim_{n\to\infty} \int \left\{ \prod_{k=1}^{n} \theta\left[\omega\left(\frac{kt}{n+1} \right) \right] \right\} P_{\mathbf{r},\mathbf{r}';t}(d\omega) \\ = \int \Omega_t(\omega) P_{\mathbf{r},\mathbf{r}';t}(d\omega). \end{aligned}$$

By definition of $P_{\mathbf{r},\mathbf{r}';t}$, the left side of this equation is identical to the right side of (2.2) for the hard-core case [cf. Eq. (2.3) below].

Having established (2.2), we use it as the rigorous starting point for our analysis. The limit $n \to \infty$ in (2.2) defines a conditional Wiener integral or path integral (conditional because both ends, $\mathbf{r}$ and $\mathbf{r}'$, are fixed). The n-fold integral in (2.2) bears to the path integral essentially the same relationship as a finite sum bears to the ordinary Riemann integral. Brush[13] has remarked that "it is usually impossible to do this" (evaluate the path integral) "by the direct method of finding an explicit formula for the finite dimensional integral and then passing to the limit of a continuous integral". Contrary to this dictum, we find, in fact, upper and lower bounds to the finite integral in (2.2) and then pass to the limit $n \to \infty$. In this way, we obtain upper and lower bounds to $G(\mathbf{r}, \mathbf{r}'; t)$.

We are interested in the case that v is a hard core, (1.12), and hence the factor $\exp[(-\Delta)v(\mathbf{z})]$ in (2.2) is equal to the simpler expression

[10] J. Ginibre, J. Math. Phys. **6**, 1432 (1965). See especially Eqs. (A1.6)–(A1.10).

[11] J. Ginibre, J. Math. Phys. **6**, 238 (1965); see the Appendix.

[12] D. Ray, Trans. Am. Math. Soc. **77**, 299 (1954).

[13] S. Brush, Rev. Mod. Phys. **33**, 79 (1961).

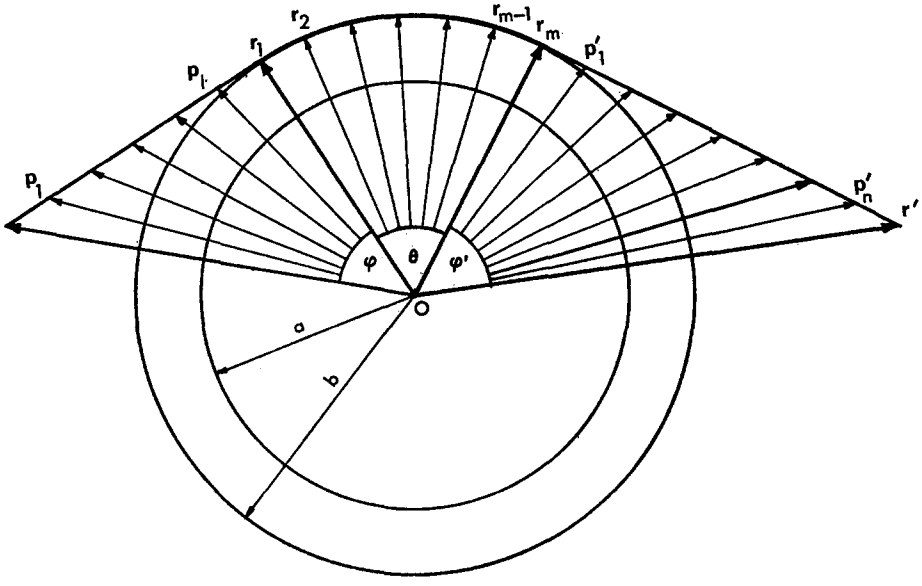

FIG. 1. Important quantities for calculating the path integral [cf. Eq. (2.9) et seq.]. The opaque sphere having radius a is shown centered at the origin, O. A slightly larger, concentric sphere of radius b is also shown. The vectors $\mathbf{r}$ and $\mathbf{r}'$ are the observation and source points, respectively, and the curve from $\mathbf{r}$ to $\mathbf{r}'$ via $\mathbf{r}_1$ and $\mathbf{r}_m$ is the shortest path from $\mathbf{r}$ to $\mathbf{r}'$ lying entirely outside the larger sphere. The straight line $\mathbf{r}_1 - \mathbf{r}$ is divided into $(l + 1)$ equal parts by the vectors $\mathbf{p}_1, \ldots, \mathbf{p}_l$; the arc θ from $\mathbf{r}_1$ to $\mathbf{r}_m$ is divided into $(m - 1)$ equal arcs by the vectors $\mathbf{r}_2, \ldots \mathbf{r}_{m-1}$; and the straight line $\mathbf{r}' - \mathbf{r}_m$ is divided to $(n + 1)$ equal parts by the vectors $\mathbf{p}_1', \ldots, \mathbf{p}_n'$.

$$\theta(\mathbf{z}) = 1, \quad \text{for} \quad z > a \qquad (2.3)$$
$$= 0, \quad \text{for} \quad z \leq a$$

for all Δ. Hence, the integrand in (2.2) is over a simple product of G_0 functions, but the integration range for each $\mathbf{z}_i$ is restricted to $z > a$. Such an integral is impossible to calculate. Since the integrand is positive, however, it is easy to obtain a lower bound to (2.2) by restricting the integration range still further, in such a manner that the restricted integral can be calculated exactly. To do this, we must define certain geometric quantities as shown in Fig. 1.

The plane of Fig. 1 is the $\mathbf{r}$, $\mathbf{r}'$ plane, and $\mathbf{0}$ is the center of the sphere of radius a. A larger, concentric sphere of radius $b > a$ is shown, and it is assumed that

$$b < \text{minimum } (r, r'). \qquad (2.4)$$

The two straight lines, $(\mathbf{r}, \mathbf{r}_1)$ and $(\mathbf{r}_m, \mathbf{r}')$, together with the circular arc $(\mathbf{r}_1, \mathbf{r}_m)$ delineate the path which would be followed by a piece of string drawn taut between $\mathbf{r}$ and $\mathbf{r}'$. Thus, $\mathbf{r}_1 \cdot (\mathbf{r} - \mathbf{r}_1) = 0$ and $\mathbf{r}_m \cdot (\mathbf{r}' - \mathbf{r}_m) = 0$. The angles φ, θ, and φ' are the angles between $\mathbf{r}$ and $\mathbf{r}_1$, $\mathbf{r}_1$ and $\mathbf{r}_m$, and $\mathbf{r}_m$ and $\mathbf{r}'$, respectively, whence

$$\psi = \varphi + \theta + \varphi' \qquad (2.5)$$

is the angle between $\mathbf{r}$ and $\mathbf{r}'$. Note that the angle θ may be zero and that the shortest path from $\mathbf{r}$ to $\mathbf{r}'$ may consist of only one straight line that does not touch the sphere of radius b. In that case $\mathbf{r}_1$ and $\mathbf{r}_n$ are not defined, but the subsequent analysis remains valid with trivial modifications. In any event,

$$S_b = r \sin \varphi + r' \sin \varphi' + b\theta \qquad (2.6)$$

is the distance from $\mathbf{r}$ to $\mathbf{r}'$ along the shortest path lying outside of a sphere of radius b.

An intuitive discussion of (2.2) is useful at this point in order to motivate the subsequent analysis. This and the following paragraph are entirely heuristic and are not part of our proof. It will be recalled that we are interested in $G(\mathbf{r}, \mathbf{r}'; t)$ for small t. In this regime, the G_0 factors in (2.2) give a large weight to that "path" (or sequences of points $\mathbf{z}_1, \cdots, \mathbf{z}_n$) from $\mathbf{r}$ to $\mathbf{r}'$ which is of shortest length. That path is, moreover, traversed with constant speed (i.e., $|\mathbf{z}_{i+1} - \mathbf{z}_i|/\Delta = \text{const}$) and is, in fact, the path of classical geometrical optics. Alternatively, we may say that a Brownian particle, which is observed to go from $\mathbf{r}$ to $\mathbf{r}'$ in a short time, most likely went by way of the Newtonian, non-Brownian, trajectory. As the time increases, the optimum path ceases to have such a preponderant weight and other paths contribute more and more to (2.2). For the case of no interaction, however, we see from (1.10) that G is *always* proportional to the maximum of the integrand, namely $\exp[-S^2/\alpha t]$, where S is the distance from $\mathbf{r}$ to $\mathbf{r}'$. When $v \neq 0$, this simple relationship will not hold for all time, but for *short time* it is clear that the "optical" path is strongly preferred *if v is finite*. Thus, for *finite* v, the factors $\exp[-\Delta v]$ in (2.2) contribute approximately the average potential along the optical path and

$$G(\mathbf{r}, \mathbf{r}'; t) \sim (\pi\alpha t)^{-\frac{3}{2}} \exp[-S^2/\alpha t]$$
$$\times \exp\left[-t \int_0^1 v(\mathbf{r} + \mu(\mathbf{r}' - \mathbf{r})\, d\mu\right]. \qquad (2.7)$$

For the hard-core case, (2.7) is patently nonsense. Instead, the fictitious Brownian particle traverses the shortest *allowed* path from $\mathbf{r}$ to $\mathbf{r}'$ with constant speed and we are thus led to the conjecture

$$G(\mathbf{r}, \mathbf{r}'; t) \sim (\pi\alpha t)^{-\frac{3}{2}} \exp\,[-S_a^2/\alpha t] \qquad (2.8)$$

for small t and for r and $r' > a$. The reason for previously introducing the slightly larger fictitious sphere of radius b is that a single path, even the optimum one, cannot by itself contribute to the integral in (2.2). The path must also be associated with a nonvanishing measure. In other words, the path must be at the center of a tube which in turn lies wholly in the allowed region. The path which just skims the surface of the sphere of radius a does not have this property, but a path of slightly greater length, lying along the larger sphere, does.

We return now to our proof. To find a lower bound we now, divide the line $(\mathbf{r}, \mathbf{r}_1)$ into $l + 1$ equal parts, designated by the vectors $\mathbf{p}_1, \cdots, \mathbf{p}_l$. Likewise, divide $(\mathbf{r}_m, \mathbf{r}')$ into $n + 1$ equal parts, designated by $\mathbf{p}_1', \cdots, \mathbf{p}_n'$. The arc $(\mathbf{r}_1, \mathbf{r}_m)$ is to be divided into $m - 1$ equal arcs, of angle $\delta = \theta/(m - 1)$, and designated by $\mathbf{r}_2, \cdots, \mathbf{r}_{m-1}$. We define

$$S_b^m = r \sin\varphi + r' \sin\varphi' + b(m - 1) \sin\delta, \qquad (2.9)$$

so that

$$S_b = \lim_{m\to\infty} S_b^m.$$

Associated with these three divisions, we define the time intervals

$$\begin{aligned} \Delta_l &= tr \sin\varphi/(l + 1)S_b^m, \\ \Delta_n &= tr' \sin\varphi'/(n + 1)S_b^m, \\ \Delta_m &= tb \sin\delta/S_b^m, \end{aligned} \qquad (2.10)$$

whence $(l + 1)\Delta_l + (m - 1)\Delta_m + (n + 1)\Delta_n = t$. Furthermore, in (2.2) let there be $l + m + n$ variables of integration and we take the limit $l, m, n \to \infty$. We make the following changes from the $\mathbf{z}_i$ variables to $\mathbf{x}_i$, $\mathbf{y}_i$, and $\mathbf{x}_i'$:

$$\begin{aligned} \mathbf{z}_i &= \mathbf{p}_i + \mathbf{x}_i \qquad (i = 1, \cdots, l), \\ \mathbf{z}_{i+l} &= \mathbf{r}_i + \mathbf{y}_i \qquad (i = 1, \cdots, m), \\ \mathbf{z}_{i+l+m} &= \mathbf{p}_i' + \mathbf{x}_i' \qquad (i = 1, \cdots, n). \end{aligned} \qquad (2.11)$$

We also use the symbol G_{lmn} to designate the integral in (2.2) before taking the limit on l, m, and n.

$$G_{lmn} = C_1 C_2 \int d\mathbf{X}\, d\mathbf{Y}\, d\mathbf{X}'\, F_1(\mathbf{X}, \mathbf{Y}, \mathbf{X}') F_2(\mathbf{Y}), \qquad (2.12)$$

where

$$C_1 = (\pi\alpha\,\Delta_l)^{-\frac{3}{2}(l+1)} (\pi\alpha\,\Delta_m)^{-\frac{3}{2}(m-1)} (\pi\alpha\,\Delta_n)^{-\frac{3}{2}(n+1)},$$

$$C_2 = \exp\left\{-\frac{S_b^m}{\alpha t}\left[r \sin\varphi + r' \sin\varphi' + 2b(m - 1)\frac{1 - \cos\delta}{\sin\delta}\right]\right\}, \qquad (2.13)$$

$$\begin{aligned} F_1(\mathbf{X}, \mathbf{Y}, \mathbf{X}') = \exp\Bigg\{ &-(\alpha\Delta_l)^{-1}\Bigg[\sum_{j=2}^{l} |\mathbf{x}_j - \mathbf{x}_{j-1}|^2 \\ &+ |\mathbf{x}_1|^2 + |\mathbf{y}_1 - \mathbf{x}_l|^2\Bigg] \\ &- (\alpha\Delta_m)^{-1} \sum_{j=2}^{m} |\mathbf{y}_j - \mathbf{y}_{j-1}|^2 \\ &- (\alpha\Delta_n)^{-1}\Bigg[\sum_{j=2}^{n} |\mathbf{x}_j' - \mathbf{x}_{j-1}'|^2 \\ &+ |\mathbf{x}_m'|^2 + |\mathbf{y}_n - \mathbf{x}_1'|^2\Bigg]\Bigg\}, \end{aligned} \qquad (2.14)$$

$$F_2(\mathbf{Y}) = \exp\left\{-\frac{2}{\alpha\Delta_m}\sum_{j=1}^{m} \mathbf{y}_j \cdot \mathbf{u}_j\right\}, \qquad (2.15)$$

with

$$\begin{aligned} \mathbf{u}_j &= 2\mathbf{r}_j - \mathbf{r}_{j-1} - \mathbf{r}_{j+1}, \quad \text{for} \quad j = 2, \cdots, m - 1, \\ \mathbf{u}_1 &= \mathbf{r}_1 - \mathbf{r}_2 + (\mathbf{r}_1 - \mathbf{r})b \sin\delta/r \sin\varphi, \\ \mathbf{u}_m &= \mathbf{r}_m - \mathbf{r}_{m-1} + (\mathbf{r}_m - \mathbf{r}')b \sin\delta/r' \sin\varphi'. \end{aligned} \qquad (2.16)$$

We come now to the important point for which Eqs. (2.9)–(2.16) were preparations. From (2.11), it is clear that, by restricting the integration variables $\mathbf{x}_i$, $\mathbf{y}_i$, and $\mathbf{x}_i'$ to the regions

$$|\mathbf{x}_i| < c, \quad |\mathbf{y}_i| < c, \quad \text{and} \quad |\mathbf{x}_i'| < c, \qquad (2.17)$$

where $c = b - a$, we can, on the one hand, satisfy the hard-sphere condition (2.3) and, on the other hand, obtain a lower bound for G_{lmn}. We also note that

$$\begin{aligned} |\mathbf{u}_i| &= 2b(1 - \cos\delta), \quad \text{for} \quad i = 2, \cdots, m - 1 \\ &= b(1 - \cos\delta), \quad \text{for} \quad i = 1 \quad \text{or} \quad m. \end{aligned} \qquad (2.18)$$

Thus, in the region, (2.17), we can replace the factor $F_2(\mathbf{Y})$ by the bound

$$\begin{aligned} F_2(\mathbf{Y}) &\geq \exp\left\{-2(\alpha\Delta_m)^{-1}\sum_{i=1}^{m} c\,|\mathbf{u}_i|\right\} \\ &= \exp\{-4c(m - 1)(1 - \cos\delta)S_b^m/\alpha t \sin\delta\} \\ &\underset{m\to\infty}{\to} \exp\{-2S_b c\theta/\alpha t\} \equiv C_3. \end{aligned} \qquad (2.19)$$

We also note that

$$\lim_{m\to\infty} C_2 = \exp\{-S_b^2/\alpha t\}. \tag{2.20}$$

We must now calculate the quantity (which is independent of $\mathbf{r}$ and $\mathbf{r}'$)

$$C_4 = C_1 \int d\mathbf{X}\, d\mathbf{Y}\, d\mathbf{X}'\, F_1(\mathbf{X}, \mathbf{Y}, \mathbf{X}'),$$

and we note that, in the limit $l, m, n \to \infty$, this is the Wiener integral for a well-known Green's function. Namely, consider the solution to (1.6) and (1.7) with zero potential but with $\mathbf{r}$ and $\mathbf{r}'$ in the *interior* of a sphere of radius c and with $G = 0$ boundary conditions on the surface of the sphere. If we denote this Green's function by $G_c(\mathbf{r}, \mathbf{r}'; t)$ then, in the limit $l, m, n \to \infty$,

$$C_4 = G_c(0, 0; t). \tag{2.21}$$

To compute G_c, it is convenient to use the expansion (1.14). Each $\psi_n(\mathbf{r})$ is a spherical harmonic times a spherical Bessel function but, since we are interested only in the point $\mathbf{r} = \mathbf{r}' = 0$, only S-wave (spherically symmetric) solutions will be relevant. For S waves, the normalized radial functions are simply $(2\pi c)^{-\frac{1}{2}} \sin kr/r$, the energies are $e(k) = \frac{1}{4}\alpha k^2$, and $k = n\pi/c$ with $n = 1, 2, 3, \cdots$. Thus,

$$C_4 = \frac{\pi}{2c^3} \sum_{n=1}^{\infty} n^2 \exp\left\{-\left(\frac{\alpha^{\frac{1}{2}}\pi}{2c}\right)^2 tn^2\right\} \tag{2.22}$$

$$> \frac{\pi}{2c^3} \exp\left\{-\left(\frac{\alpha^{\frac{1}{2}}\pi}{2c}\right)^2 t\right\}. \tag{2.23}$$

Our lower bound for $G(\mathbf{r}, \mathbf{r}'; t)$ is the product of C_2, C_3, and C_4, each of which depends on $\mathbf{r}$ and $\mathbf{r}'$ and/or the radius b (or $c = b - a$):

$$G(\mathbf{r}, \mathbf{r}'; t) > \frac{\pi}{2c^3} \exp\left\{-\frac{S_b^2 + 2S_b c\theta}{\alpha t} - \left(\frac{\alpha^{\frac{1}{2}}\pi}{2c}\right)^2 t\right\}. \tag{2.24}$$

The inequality (2.24) is generally valid, even if the geodesic from $\mathbf{r}$ to $\mathbf{r}'$ around the sphere of radius b is a straight line. In that case the term $2S_b c\theta/\alpha t$ is to be omitted.

The next step is to determine c so that the right-hand side of (2.24) is maximized. This is a tedious problem since the dependence of S_b on c is complicated. Furthermore, b must always be less than r and r'. To calculate B_{exch}, however, we are interested in having $\mathbf{r} = -\mathbf{r}'$ and, from (1.4), it is clear that $r \sim a$ is the important region to consider in the integral. For our purpose—the proof of (1.13)—it is sufficient, as well as legitimate, to take $c = r - a$. The distance S_b is then simply πr, while θ is simply π for all $r > a$.

Thus,

$$\frac{B_{\text{exch}}}{B^0_{\text{exch}}} = 8 \int G(\mathbf{r}, -\mathbf{r}; 2\Lambda^2/\pi\alpha)\, d\mathbf{r}$$

$$> 8 \int_a^\infty 4\pi r^2\, dr \frac{\pi}{2(r-a)^3} \times \exp\left\{-\pi^3 \frac{r^2 + 2r(r-a)}{2\Lambda^2} - \frac{\pi\Lambda^2}{2(r-a)^2}\right\}$$

$$> 4\pi^2\Omega^4 e^{-\frac{1}{2}\pi^3(a/\Lambda)^3} \int_0^\infty \frac{dp}{p^3} \times \exp\left\{-\frac{\pi^2}{2}\left[3\frac{p^2}{\Omega} + \Omega\left(2p + \frac{1}{p^2}\right)\right]\right\}, \tag{2.25}$$

where

$$\Omega = (4\pi)^{\frac{1}{3}}(a/\Lambda)^{\frac{2}{3}}. \tag{2.26}$$

The second inequality in (2.25) is obtained by noting that $r^2 \geq a^2$, and by changing variables to $p = (2\pi^2)^{1/3}\Lambda^{-4/3}a^{1/3}(r - a)$.

The inequality (2.25) is plainly of the form stated in (1.13). To make it more definite, however, we can obtain a lower bound to the integral in (2.25) in the following way: Replace the integration region by (0, 1) instead of (0, ∞); in this region, the terms p^2 and p in the exponent may be replaced by unity. We are thus left with an integral of the form $\int_0^1 dp p^{-3} \cdot \exp(-\frac{1}{2}\pi^2\Omega p^{-2}) = (\pi^2\Omega)^{-1} \exp(-\frac{1}{2}\pi^2\Omega)$. Collecting the various factors, we obtain

$$\frac{B_{\text{exch}}}{B^0_{\text{exch}}} > \exp\left\{-\frac{\pi^3}{2}\left(\frac{a}{\Lambda}\right)^2 - \frac{3\pi^2}{2}\left(2\sqrt{\pi}\,\frac{a}{\Lambda}\right)^{\frac{2}{3}} + 2\ln\left(4\sqrt{\pi}\,\frac{a}{\Lambda}\right) - \frac{3\pi^2}{2}\left(2\sqrt{\pi}\,\frac{a}{\Lambda}\right)^{-\frac{2}{3}}\right\} \tag{2.27}$$

as our final lower bound for B_{exch}.

III. UPPER BOUND BY PATH INTEGRALS

We are interested in computing the path integral, (2.2), when the factors $\exp[-\Delta v(\mathbf{z})]$ are omitted, but when the integration ranges are restricted to $|z_i| > a$ for all i. The lower bound to (2.2) was obtained in Sec. II by restricting the integration range still further, namely, to a tube lying just outside the sphere. At first sight it would seem that the opposite procedure—integrating over too great

a region—should yield a suitable upper bound. Indeed, when $\mathbf{r}$ and $\mathbf{r}'$ are in each other's *line of sight* (i.e., when the straight line between the two points does not interest the sphere), then the simple expedient of integrating over *all* space yields an upper bound which is at once useful and accurate for small time (high temperature), viz:

$$G(\mathbf{r}, \mathbf{r}'; t) < G_0(\mathbf{r}, \mathbf{r}'; t). \tag{3.1}$$

While (3.1) is true for all $\mathbf{r}$ and $\mathbf{r}'$, it is quite misleading when the two points are in each other's *shadow*. A more sensitive extension of the integration range is required; but, unfortunately, allowing the paths to penetrate the sphere only slightly does not render the integral any more tractable than the original. In order to make the integration feasible, it appears to be necessary to extend the integrations to all space; but then the upper bound so obtained, (3.1), is virtually useless.

Our resolution of the dilemma is to integrate over all space, but at the same time to include an additional weight factor in the integrand of (2.2) so that paths which penetrate the sphere are effectively suppressed.

As in Sec. II, we consider the "taut string" shown in Fig. 1, except that this time we take $c = 0$ (i.e., radius b = radius a). Otherwise, everything is the same as given in Eqs. (2.10)–(2.16). The first step in obtaining an upper bound is to integrate over the variables $\mathbf{X}$ and $\mathbf{X}'$ (alternatively, $\mathbf{z}_i$ for $i=1, \cdots, l$ and $i=l+m+1, \cdots, l+m+n$) over *all* space. We then pass to the limit l and $n \to \infty$ and obtain

$$G(\mathbf{r}, \mathbf{r}'; t) < \lim_{m\to\infty} G_m(\mathbf{r}, \mathbf{r}'; t), \tag{3.2}$$

where

$$G_m(\mathbf{r}, \mathbf{r}'; t) = D_1 C_2 \int_R d\mathbf{Y}\, F_2(\mathbf{Y}) F_3(\mathbf{Y}), \tag{3.3}$$

with

$$D_1 = (\pi\alpha t_1)^{-\frac{3}{2}} (\pi\alpha t_2)^{-\frac{3}{2}} (\pi\alpha\Delta_m)^{-\frac{3}{2}(m-1)}, \tag{3.4}$$

$$F_3(\mathbf{Y}) = \exp\left\{-(\alpha t_1)^{-1} |\mathbf{y}_1|^2 - (\alpha t_2)^{-1} |\mathbf{y}_m|^2 - (\alpha\Delta_m)^{-1} \sum_{i=2}^{m} |\mathbf{y}_i - \mathbf{y}_{i-1}|^2\right\}, \tag{3.5}$$

and

$$t_1 = (l+1)\,\Delta_l = tr \sin\varphi / S_a^m, \qquad t_2 = (n+1)\,\Delta_n = tr' \sin\varphi' / S_a^m. \tag{3.6}$$

The quantities C_2 and F_2 are as given in (2.13) and (2.15), respectively (with $b = a$, of course).

The integration range in (3.3) is

$$R\colon |\mathbf{y}_i + \mathbf{r}_i| > a, \quad \text{for} \quad i = 1, \cdots, m. \tag{3.7}$$

Since the $\mathbf{r}_i$ are different, one from another, the integration range for each i is different. To overcome this complication, we integrate (3.3) over all space *after* first replacing the function $F_2(\mathbf{Y})$ by another positive function, $\bar{F}_2(\mathbf{Y})$, which has the property that $\bar{F}_2(\mathbf{Y}) \geq F_2(\mathbf{Y})$ for $\mathbf{Y}$ in the allowed region, R, while $\bar{F}_2(\mathbf{Y})$ is generally less than $F_2(\mathbf{Y})$ for paths which penetrate the sphere. First note that the vectors $\mathbf{u}_i$, given in (2.16), are parallel to $\mathbf{r}_i$:

$$\begin{aligned} \mathbf{u}_i &= 2(1 - \cos\delta)\mathbf{r}_i, \quad \text{for} \quad i = 2, \cdots, m-1 \\ &= (1 - \cos\delta)\mathbf{r}_i, \quad \text{for} \quad i = 1 \quad \text{or} \quad m. \end{aligned} \tag{3.8}$$

In the allowed region, R, we have $a^2 \leq |\mathbf{y}_i + \mathbf{r}_i|^2 = |\mathbf{y}_i|^2 + 2\mathbf{y}_i\cdot\mathbf{r}_i + a^2$. Thus, in R,

$$\begin{aligned} \mathbf{y}_i\cdot\mathbf{u}_i &\geq -|\mathbf{y}_i|^2 (1 - \cos\delta), \\ &\qquad \text{for} \quad i = 2, \cdots, m-1 \\ &\geq -\tfrac{1}{2} |\mathbf{y}_i|^2 (1 - \cos\delta), \\ &\qquad \text{for} \quad i = 1 \quad \text{or} \quad m. \end{aligned} \tag{3.9}$$

Hence, in, R

$$F_2(\mathbf{Y}) \leq \bar{F}_2(\mathbf{Y}) = \exp\left\{\frac{1 - \cos\delta}{\alpha\,\Delta_m} \times \left[|\mathbf{y}_i|^2 + |\mathbf{y}_m|^2 + 2\sum_{i=2}^{m-1} |\mathbf{y}_i|^2\right]\right\}. \tag{3.10}$$

Now, the integral over all space of the product $\bar{F}_2(\mathbf{Y})F_3(\mathbf{Y})$ is a simple m-dimensional Gaussian integral, which can be evaluated by using the well-known formula

$$\int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_N \exp\left\{-\sum_{i,j=1}^{N} x_i A_{ij} x_j\right\} = \pi^{N/2} [\mathrm{Det}\, A]^{-\frac{1}{2}}, \tag{3.11}$$

for any symmetric, positive definite N-square matrix A. Applying this formula to G_m (with F_2 replaced by $\bar{F}_2$), we obtain

$$G_m(\mathbf{r}, \mathbf{r}'; t) < C_2 \left[\frac{\pi\,\alpha t_1 t_2}{\Delta_m} |B^m|\right]^{-\frac{3}{2}}, \tag{3.12}$$

where $|B^m|$ is the determinant of the tri-diagonal m-square matrix

$$B^m = \begin{bmatrix} \frac{\Delta_m}{t_1} + \cos\delta & -1 & & & & & \\ -1 & 2\cos\delta & -1 & & & 0 & \\ & -1 & 2\cos\delta & -1 & & & \\ & & -1 & \ddots & \ddots & & \\ & & & \ddots & \ddots & -1 & \\ & & 0 & & -1 & 2\cos\delta & -1 \\ & & & & & -1 & \frac{\Delta_m}{t_2} + \cos\delta \end{bmatrix}. \tag{3.13}$$

The exponent $\frac{3}{2}$ in (3.12) instead of $\frac{1}{2}$ as in (3.11) comes about because each of the m variables of integration is three dimensional.

In order for (3.12) to be valid, it is necessary that B_m be positive definite. If $\delta = 0$, that criterion is surely satisfied and (by continuity) B_m is positive definite for $0 < \delta < \bar{\delta}$, where $\bar{\delta}$ is the smallest value of δ for which $|B^m| = 0$.

To evaluate $|B^m|$, we expand in the first row and column as well as in the mth row and column and obtain

$$|B^m| = \left(\cos\delta + \frac{\Delta_m}{t_1}\right)\left(\cos\delta + \frac{\Delta_m}{t_2}\right)U_{m-2} - \left(2\cos\delta + \frac{\Delta_m}{t_1} + \frac{\Delta_m}{t_2}\right)U_{m-3} + U_{m-4}, \tag{3.14}$$

where U_m is the m-square determinant

$$U_m = \mathrm{Det}\begin{bmatrix} 2\cos\delta & -1 & & & & \\ -1 & 2\cos\delta & -1 & & 0 & \\ & -1 & 2\cos\delta & -1 & & \\ & & -1 & \ddots & \ddots & \\ & 0 & & \ddots & \ddots & -1 \\ & & & & -1 & 2\cos\delta \end{bmatrix}. \tag{3.15}$$

Since U_m obviously satisfies the recursion relationship

$$U_m = 2\cos\delta U_{m-1} - U_{m-2}, \tag{3.16}$$

it follows that U_m ($\cos\delta$) is the Chebyshev polynominal of the second kind[14] (in the variable $\cos\delta$), whence

$$U_m = \sin(m+1)\,\delta/\sin\delta. \tag{3.17}$$

Combining (3.17) with (3.14) and, recalling that $\theta = (m-1)\delta$, we obtain

$$|B^m| = \frac{\Delta_m^2 \sin\theta}{t_1 t_2 \sin\delta} - \Delta_m\left(\frac{1}{t_1} + \frac{1}{t_2}\right)\cos\theta - \sin\theta\sin\delta. \tag{3.18}$$

Now, recalling the definitions (2.10), (3.6) and the fact that $r\cos\varphi = a = r'\cos\varphi'$, (3.18) is equivalent to

$$\frac{t_1 t_2}{\Delta_m}|B^m| = \frac{ta\sin(\varphi + \varphi' + \theta)}{S_a^m \cos\varphi\cos\varphi'}. \tag{3.19}$$

But $\varphi + \varphi' + \theta = \psi$ = angle between $\mathbf{r}$ and $\mathbf{r}'$ [cf. (2.5)]. Thus, combining (3.19) with (2.13), (3.3), and (3.12) and passing to the limit $m \to \infty$, we have our upper bound

$$G(\mathbf{r}, \mathbf{r}'; t) < \left[\frac{S_a\cos\varphi\cos\varphi'}{\pi\alpha t a\sin\psi}\right]^{\frac{3}{2}} \exp\left\{-\frac{S_a^2}{\alpha t}\right\}. \tag{3.20}$$

[14] A. Erdelyi, Ed., *Higher Transcendental Functions* (McGraw-Hill Book Co., Inc., New York, 1953), Vol. II, Chap. 10, p. 183.

Formula (3.20) has the essential feature that we have sought, namely, the factor exp $\{-(\text{shortest distance from } \mathbf{r} \text{ to } \mathbf{r}' \text{ around the sphere})^2/\alpha t\}$. It also has the factor $(\pi\alpha t)^{-\frac{3}{2}}$, characteristic of G_0. The factor $(S_a \cos\varphi \cos\varphi'/a \sin\psi)$, while it is usually of the order of unity, can be embarrassingly large when $\psi \sim \pi$. Unfortunately, it is precisely the case of diametric juxtaposition of $\mathbf{r}$ and $\mathbf{r}'$ that is of interest in calculating B_{exch}. Plainly, some slight improvement is required before inserting (3.20) into (1.4).

It is interesting to note, however, that the divergence in our upper bound at $\psi = \pi$ is not entirely unexpected. This is because many paths of the *same length* come together at that angle. In other words, $\psi = \pi$ can be regarded as a caustic. Our upper bound concentrated essentially on only one path around the sphere and, since that one path is not sufficient at $\psi = \pi$, difficulties were encountered there. It is noteworthy that precisely the same divergence is encountered in the classical asymptotic expansion for diffraction around a sphere.[7]

A simple artifice to overcome the annoying $(\sin\psi)^{-\frac{3}{2}}$ factor is the following: Let $\mathbf{OQ}$ be a vector of length $q < a$ perpendicular to $\mathbf{r}$ and let s' be the sphere of radius $b = a - q$ centered at the point Q. This sphere is clearly tangent to the original sphere, s, (of radius a) at the single point $(a/q)\mathbf{OQ}$ and otherwise lies entirely inside the larger sphere, s. Also, let $G_{s'}(\mathbf{r}, \mathbf{r}'; t)$ be the Green's function for the exterior of s', just as $G(\mathbf{r}, \mathbf{r}'; t)$ is the Green's function for the exterior of s. From (2.2), we see at once,

$$G(\mathbf{r}, \mathbf{r}'; t) < G_{s'}(\mathbf{r}, \mathbf{r}'; t) \tag{3.21}$$

for all points $\mathbf{r}$ and $\mathbf{r}'$. We can, in turn, say that $G_{s'}$ is less than the right-hand side of (3.20), where the quantities φ, φ', ψ, and S are now measured relative to the sphere s' centered at Q.

For our purposes, we want $\mathbf{r}' = -\mathbf{r}$ with $r > a$. Relative to the sphere s', we have the following simple geometric inequalities for all $r > a$:

$$\begin{aligned} &\pi(a - 3q) < S < \pi r, \\ &\sin\psi = \frac{2rq}{r^2 + q^2} > \frac{q}{r}. \end{aligned} \tag{3.22}$$

In addition, $\cos\varphi \cos\varphi' < 1$, whence

$$G(\mathbf{r}, -\mathbf{r}; t) < r^3(\alpha t a q)^{-\frac{3}{2}} \times \exp\{-\pi^2(a - 3q)^2/\alpha t\}, \tag{3.23}$$

for any $0 < q < a/3$ and for all $r > a$.

We can now evaluate B_{exch} as given by (1.4). To do so, we divide the integration range $\int_a^\infty dr$ into two parts: $\int_a^{2a} dr$ and $\int_{2a}^\infty dr$. In the former range, we use the bound (3.23), while in the later range, we use the very simple bound G_0 as in (3.1). Thus,

$$\begin{aligned} \frac{B_{\text{exch}}}{B^0_{\text{exch}}} &= 8\int G(\mathbf{r}, -\mathbf{r}; 2\Lambda^2/\pi\alpha)\, d\mathbf{r} \\ &< 8\int_a^{2a} dr\, 4\pi r^2 r^3 [2\Lambda^2 q a/\pi]^{-\frac{3}{2}} \\ &\qquad \times \exp\{-\pi^3(a - 3q)^2/2\Lambda^2\} \\ &\quad + 8\int_{2a}^\infty dr\, 4\pi r^2 (2\Lambda^2)^{-\frac{3}{2}} \exp\{-2\pi r^2/\Lambda^2\}. \end{aligned} \tag{3.24}$$

In the first integral, take $q = \Lambda^2/(2\pi^3 a)$, assuming that $(\Lambda/a)^2 < 2\pi^3/3$. The second integral is clearly Order $\{\exp[-8\pi(a/\Lambda)^2]\}$ and is therefore exponentially small compared to $\exp[-\frac{1}{2}\pi^3(a/\Lambda)^2]$. While an upper bound to this second terms can be easily found, there is little point in doing so.

Evaluating the first integral in (3.24) and combining it with the second, we obtain our final upper bound:

$$\frac{B_{\text{exch}}}{B^0_{\text{exch}}} < \exp\left\{-\frac{\pi^3}{2}\left(\frac{a}{\Lambda}\right)^2 + \ln\left[\frac{1}{3}\, 2^{10}\pi^7\left(\frac{a}{\Lambda}\right)^6\right] + \frac{3}{2} - \frac{9}{(2\pi)^3}\left(\frac{\Lambda}{a}\right)^2 + O\left[\exp\left(\tfrac{1}{2}\pi^3 - 8\pi\right)\left(\frac{a}{\Lambda}\right)^2\right]\right\}. \tag{3.25}$$

IV. CONCLUSIONS

By means of the discrete version of the Wiener integral, (2.2), we have obtained upper and lower bounds to the diffusion Green's function in the presence of an opaque sphere [Eqs. (2.24) and (3.20), respectively]. These bounds are useful for short time (high temperature), especially when the source point and the observation point are in each other's shadow.

The bounds enable us to calculate lower and upper bounds to the exchange part of the second virial coefficient of a hard-sphere gas. These bounds, respectively, given in (2.27) and (3.25), permit us to assert that the correct B_{exch} diminishes with temperature much more rapidly than the non-interacting B^0_{exch}, in a manner given by the equation

$$\frac{B_{\text{exch}}}{B^0_{\text{exch}}} = \exp\left\{-\frac{\pi^3}{2}\left(\frac{a}{\Lambda}\right)^2 + O\left[\left(\frac{a}{\Lambda}\right)^{\frac{3}{2}}\right]\right\}.$$

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Generalization of the Variational Method of Kahan, Rideau, and Roussopoulos. II. A Variational Principle for Linear Operators and its Application to Neutron-Transport Theory*

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Additional applications of a generalized form of the variational method of Kahan, Rideau, and Roussopoulos are presented. Equations used in neutron transport theory, such as the spherical harmonics operator form of the Boltzmann equation, are derived from the generalized variational functional and an interpretation of these operator equations in terms of flux- and source-generating operators is suggested. A relationship between this variational method and the variational method of Lippmann and Schwinger is established, and it is shown that the least-squares variational functional of Becker for linear equations can be derived from a generalized variational functional.

1. INTRODUCTION

AMONG the many applications of variational methods are the derivations of exact and approximate equations of mathematical physics and estimations of eigenvalues and weighted averages. In neutron transport theory, for example, variational techniques have been used to calculate the asymptotic and nonasymptotic neutron density for the Milne problem,[1,2] to estimate the condition of criticality,[3] to treat resonance escape probabilities,[4] and to deal with thermalization and space–energy problems.[5]

It is the purpose of this paper to develop further a generalized form of the variational method of Kahan, Rideau, and Roussopoulos[6–8] discussed previously,[9] and to present additional applications. By investigating trial operators $G_T(t, t')$ that are explicit functions of two variables, we show a connection with the variational method of Lippmann and Schwinger. The least-squares variational method of Becker for linear operators and approximate neutron transport operator equations, with their interpretations in terms of flux- and source-generating operators, are derived from a generalized variational method.

Let us consider the linear equations

$$\int L(t, t'')G(t'', t')\,dt'' = I\,\delta(t - t') = \int G(t, t'')L(t'', t')\,dt'', \quad (1)$$

where I is the identity operator and the specified linear operator $L(t, t')$ and the desired Green's operator $G(t, t')$ depend on the variables t and t'. We wish to construct a variational expression $G_v(t, t')$ for the Green's operator $G(t, t')$, where G_v is a function of the trial Green's operators $G_1(t, t')$ and $G_2(t, t')$. Following the procedure described in I, we readily obtain the desired variational expression:

$$G_v(t, t') = G_1(t, t') + G_2(t, t') - \iint G_1(t, t'')L(t'', t''')G_2(t''', t')\,dt''\,dt'''. \quad (2)$$

This equation may be considered as a particular form of the linear operators occurring in (I.34) with the dependence of the operators on t and t' being explicitly noted. As shown in I, first-order variations in the trial operators G_1 and G_2 about the exact Green's operator G result in second-order variations in G_v about G.

2. RELATED VARIATIONAL EXPRESSIONS

A relationship between the variational expression (2) and the Lippmann–Schwinger variational princi-

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[1] R. E. Marshak, Phys. Rev. **71**, 688 (1947).
[2] J. LeCaine, Phys. Rev. **72**, 564 (1947).
[3] A. M. Weinberg and E. P. Wigner, *The Physical Theory of Neutron Chain Reactors* (The University of Chicago Press, Chicago, Illinois, 1958).
[4] N. Corngold, Proc. Phys. Soc. (London) **A70**, 793 (1957).
[5] N. C. Francis, J. C. Stewart, L. S. Bohl, and T. J. Krieger, Progr. Nucl. Energy, Ser. I **3**, 360 (1959).
[6] T. Kahan and G. Rideau, Compt. Rend. **233**, 849 (1951).
[7] T. Kahan and G. Rideau, J. Phys. Radium **13**, 326 (1952).
[8] P. Roussopoulos, Compt. Rend. **236**, 1858 (1953).
[9] M. D. Kostin and H. Brooks, J. Math. Phys. **5**, 1691 (1964), hereafter referred to as I.

ple for the collision operator,[10] used in nuclear scattering theory, can be shown by setting

$$L(t, t') = -iH(t)\,\delta(t - t') + H(t)\eta(t - t')H(t'), \quad (3)$$

where $H(t)$ is the interaction Hamiltonian, Planck's constant $\hbar = 1$, and $\eta(t - t')$ is the step function

$$\begin{aligned} \eta(t - t') &= 1, \quad \text{for} \quad t > t' \\ &= 0, \quad \text{for} \quad t < t'. \end{aligned} \quad (4)$$

The collision operator S, expressed in terms of the Green's operator, has the form

$$S = I - i \iint H(t)G(t, t')H(t')\,dt\,dt', \quad (5)$$

where the range of integration extends from $-\infty$ to $+\infty$. Substituting (3) into the variational expression (2) for the operator $\iint H(t)G(t, t')H(t')\,dt\,dt'$ we obtain

$$\begin{aligned} S_s = I &- i \int [H(t)A_T(t) \\ &+ B_T(t)H(t) - B_T(t)H(t)A_T(t)]\,dt \\ &- \iint B_T(t)H(t)\eta(t - t')H(t')A_T(t')\,dt\,dt', \end{aligned} \quad (6)$$

where the trial operators A_T and B_T are related to trial Green's operators by the equations

$$A_T(t) = \int G_2(t, t')H(t')\,dt', \quad (7)$$

$$B_T(t) = \int H(t')G_1(t', t)\,dt'. \quad (8)$$

Equation (6) is recognized as the Lippmann–Schwinger variational principle for the collision operator S, where A_T and B_T are trial operators for the unitary operators U_+ and $U_-^\dagger$, respectively.

The least-squares variational functional of Becker[11]

$$j_b = \int (Lf_T - s)^2 p(x)\,dx \quad (9)$$

for the linear equation $Lf = s$, where $p(x)$ is Becker's positive weighting function, can be derived from the generalized variational functional

$$j = (w, [G_1 + G_2 - G_1LG_2]s) \quad (10)$$

by defining the scalar product to include the weighting function:

$$(g, f) = \int g(x)f(x)p(x)\,dx. \quad (11)$$

Let $w = L^\dagger s$, let the trial operator G_2 generate the trial function $f_T = G_2 s$, and let the remaining trial operator be formally given by $G_1^\dagger = LG_2G^\dagger$. The variational functional (10) now becomes

$$\begin{aligned} j &= 2(s, Lf_T) - (Lf_T, Lf_T) \\ &= (s, s) - (Lf_T - s, Lf_T - s) \\ &= (s, s) - j_b, \end{aligned} \quad (12)$$

which is equivalent to Becker's variational functional.

3. A DERIVATION OF OPERATOR EQUATIONS FROM A VARIATIONAL PRINCIPLE

In addition to its applications for estimating weighted averages and eigenvalues, the variational principle has been used to derive systematically approximate equations of reactor theory. Calame and Brooks[12,13] have derived the multigroup equations from a variational principle. Selengut[14] and Rowlands[15] have discussed the reduction of neutron transport equations involving many independent variables to simpler equations with fewer independent variables. Boundary terms in the variational principle have been investigated by Federighi.[16] These contributions are extended in this section. Here the variational operator method is used to derive an approximate system of operator equations, a procedure which leads us to an interpretation of the variational formalism.

For definiteness we consider a problem with two independent variables such as the one-velocity, plane-geometry Boltzmann integro-differential equation with isotropic scattering:

$$\begin{aligned} u \frac{\partial}{\partial z} g(z, u; z_s, u_s) &+ \Sigma\, g(z, u; z_s, u_s) \\ &- \tfrac{1}{2}\,\Sigma_s \int_{-1}^{+1} du'\, g(z, u'; z_s, u_s) \\ &= \delta(z - z_s)\,\delta(u - u_s). \end{aligned} \quad (13)$$

Using the variational operator functional

$$j[G_1, G_2] = (w, [G_1 + G_2 - G_1LG_2]s), \quad (14)$$

[10] B. A. Lippmann and J. Schwinger, Phys. Rev. 79, 469 (1950).

[11] M. Becker, *The Principles and Applications of Variational Methods* (Technology Press, Cambridge, Massachusetts, 1964).

[12] G. P. Calame and H. Brooks, Trans. Am. Nucl. Soc. 2, 56 (1959).

[13] G. P. Calame, Ph.D. thesis, Harvard University (1959).

[14] D. S. Selengut, Trans. Am. Nucl. Soc. 2, 58 (1959); Hanford Laboratories Rept. HW-59126 (1959).

[15] G. Rowlands, J. Nucl. Energy 13, 176 (1961).

[16] F. D. Federighi, Ph.D. thesis, Harvard University (1961).

we introduce the trial operators

$$G_1 = \sum_{ij} P_{ij}B_{ij}, \tag{15}$$

$$G_2 = \sum_{ij} A_{ij}P_{ij}, \tag{16}$$

where P_{ij} are projection operators that operate on functions of the angular variable u:

$$\begin{aligned} P_{ij}s(z, u) &= p_i(u) \int_{-1}^{+1} q_j(u')s(z, u')\, du' \\ &= p_i(u)s_j(z). \end{aligned} \tag{17}$$

The unspecified operators A_{ij} and B_{ij} which act on functions of the spatial variable z are determined by the variational conditions

$$\delta j = 0 \quad \text{for arbitrary} \quad \delta A_{ij}, \tag{18}$$

$$\delta j = 0 \quad \text{for arbitrary} \quad \delta B_{ij}. \tag{19}$$

In the Boltzmann equation (13) we let the mode functions[3] $p_i(u)$ and $q_i(u)$ be the normalized Legendre polynomials

$$\begin{aligned} p_0(u) &= (\tfrac{1}{2})^{\frac{1}{2}}, & p_1(u) &= (\tfrac{3}{2})^{\frac{1}{2}}u, \\ p_2(u) &= (\tfrac{5}{8})^{\frac{1}{2}}(3u^2 - 1), & p_3(u) &= (\tfrac{7}{8})^{\frac{1}{2}}(5u^3 - 3u), \\ q_i(u) &= p_i(u), & \int_{-1}^{+1} q_i(u)p_j(u)\, du &= \delta_{ij}. \end{aligned} \tag{20}$$

All the angular dependence of the trial operators G_1 and G_2 is contained in the projection operators P_{ij}; the unspecified operators A_{ij} and B_{ij} are responsible for the spatial dependence.

The variational functional (14) with the trial operators (15) and (16) reduces to

$$\begin{aligned} j = \sum_{ij} (w_i, B_{ij}s_j) + \sum_{ij} (w_i, A_{ij}s_j) \\ - \sum_{ijkm} (w_i, B_{ij}L_{jk}A_{km}s_m), \end{aligned} \tag{21}$$

where

$$s_j(z) = \int_{-1}^{+1} q_j(u')s(z, u')\, du', \tag{22}$$

$$w_i(z) = \int_{-1}^{+1} w(z, u')p_i(u')\, du', \tag{23}$$

are functions of z and

$$L_{jk} = \int_{-1}^{+1} du\; q_j(u)Lp_k \tag{24}$$

is an operator which acts on functions of z.

The requirement $\delta j = 0$ is satisfied for arbitrary δB_{ij} if

$$\sum_k L_{jk}A_{km} = I\, \delta_{jm}, \tag{25}$$

and $\delta j = 0$ for arbitrary δA_{km} if

$$\sum_j B_{ij}L_{jk} = I\, \delta_{ik}. \tag{26}$$

If we premultiply (25) by B_{ij}, sum over j, and use (26), we see that

$$\begin{aligned} \sum_{jk} B_{ij}L_{jk}A_{km} &= \sum_j B_{ij}\, \delta_{jm}, \\ \sum_k \delta_{ik}A_{km} &= B_{im}, \\ A_{im} &= B_{im}, \end{aligned} \tag{27}$$

as expected. Moreover, on combining (21) and (26) we get

$$j = \sum_{ij} (w_i, A_{ij}s_j), \tag{28}$$

where the flux-generating operators A_{ij} are given by (25).

The term $(w_i, A_{ij}s_j)$ appearing in (28) has the following interpretation. The neutron source $s_j(z)$ in angular mode j is acted upon by the flux-generating operator (FGO) A_{ij} which produces a neutron flux $f_i(z)$ in angular mode i:

$$f_i(z) = A_{ij}s_j(z). \tag{29}$$

This flux is then absorbed by the weighting function $w_i(z)$ in angular mode i:

$$(w_i, A_{ij}s_j) = (w_i, f_i) = \int w_i(z)f_i(z)\, dz. \tag{30}$$

In order to evaluate (28), the matrix operator equation $LA = I$, which is equivalent to (25), is solved. The elements of L and A are operators:

$$L = \begin{vmatrix} L_{00} & L_{01} & \cdots \\ L_{10} & L_{11} & \\ \vdots & & \end{vmatrix} \qquad A = \begin{vmatrix} A_{00} & A_{01} & \cdots \\ A_{10} & A_{11} & \\ \vdots & & \end{vmatrix}. \tag{31}$$

If we consider the case where L is a 2-by-2 matrix, then

$$\begin{aligned} A &= \begin{vmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{vmatrix} \\ &= \begin{vmatrix} L_{00}^{-1} - L_{00}^{-1}L_{01}K_{11}^{-1}L_{10}L_{00}^{-1} & -L_{00}^{-1}L_{01}K_{11}^{-1} \\ K_{11}^{-1}L_{10}L_{00}^{-1} & K_{11}^{-1} \end{vmatrix}, \end{aligned} \tag{32}$$

where

$$K_{11} = L_{11} - L_{10}L_{00}^{-1}L_{01}. \tag{33}$$

The source-generating operator (SGO) L_{ij} generates a source in angular mode i from a flux in angular mode j:

$$s_i(z) = L_{ij}f_j(z). \tag{34}$$

In going from mode 1 to mode 1, we must take into account the presence of mode 0. The total mode-1-to-mode-1 SGO $K_{11} = L_{11} - L_{10}L_{00}^{-1}L_{01}$ includes the direct mode-1-to-mode-1 SGO L_{11} as well as the SGO $L_{10}L_{00}^{-1}L_{01}$ resulting from the existence of mode 0. L_{00}^{-1} is to be interpreted as the mode-0-to-mode-0 FGO neglecting all modes greater than 0. Similarly K_{11}^{-1} is the mode-1-to-mode-1 FGO neglecting all modes greater than 1. All the elements of (32) can be given analogous interpretations.

Another form of the FGO matrix A is obtained by interchanging the roles played by the two modes,

$$A = \begin{vmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{vmatrix} = \begin{vmatrix} K_{00}^{-1} & -K_{00}^{-1}L_{01}L_{11}^{-1} \\ -L_{11}^{-1}L_{10}K_{00}^{-1} & L_{11}^{-1} - L_{11}^{-1}L_{10}K_{00}^{-1}L_{01}L_{11}^{-1} \end{vmatrix}, \tag{35}$$

where

$$K_{00} = L_{00} - L_{01}L_{11}^{-1}L_{10} \tag{36}$$

is the mode-0-to-mode-0 SGO neglecting all modes except 0 and 1.

Let us apply this formalism to the Boltzmann equation (13), which has the source-generating operator

$$Lf(z, u) = u\frac{\partial}{\partial z}f(z, u) + \Sigma f(z, u) - \tfrac{1}{2}\Sigma_s \int_{-1}^{+1} du' f(z, u'). \tag{37}$$

Using the normalized Legendre polynomials (20) with (24), we obtain an explicit result for the matrix operator L in (31):

$$L = \begin{vmatrix} (\Sigma - \Sigma_s)I & \frac{1}{3^{\frac{1}{2}}}D & 0 & 0 & & & 0 \\ \frac{1}{3^{\frac{1}{2}}}D & \Sigma I & \frac{2}{(15)^{\frac{1}{2}}}D & 0 & & & 0 \\ 0 & \frac{2}{(15)^{\frac{1}{2}}}D & \Sigma I & \frac{3}{(35)^{\frac{1}{2}}}D & & & 0 \\ 0 & 0 & \frac{3}{(35)^{\frac{1}{2}}}D & \Sigma I & & & \\ & & & & \Sigma I & \frac{n+1}{[(2n+1)(2n+3)]^{\frac{1}{2}}}D & \\ 0 & & 0 & & \frac{n+1}{[(2n+1)(2n+3)]^{\frac{1}{2}}}D & \Sigma I & \end{vmatrix}, \tag{38}$$

where D is the spatial differential operator d/dz, and I is the identity operator. Here (25) becomes the matrix operator form of the spherical harmonics method for plane geometry.

Let us consider only modes 0 and 1, and neglect all higher modes so that the matrix operator L simplifies to

$$L = \begin{vmatrix} (\Sigma - \Sigma_s)I & (\frac{1}{3})^{\frac{1}{2}}D \\ (\frac{1}{3})^{\frac{1}{2}}D & \Sigma I \end{vmatrix}. \tag{39}$$

Suppose that $s_1(x) = 0$ and $w_1(x) = 0$ so that (28) reduces to

$$j = (w_0, A_{00}s_0), \tag{40}$$

where the flux-generating operator A_{00} is given in (35):

$$A_{00} = K_{00}^{-1} = [L_{00} - L_{01}L_{11}^{-1}L_{10}]^{-1} \tag{41}$$

or

$$[L_{00} - L_{01}L_{11}^{-1}L_{10}]A_{00} = I. \tag{42}$$

Equation (42) has the form

$$\left[[\Sigma - \Sigma_s] - \frac{1}{3\Sigma}\frac{d^2}{dz^2}\right]A_{00}(z, z_s) = \delta(z - z_s), \tag{43}$$

which we recognize as the equation for the Green's function given by the diffusion theory approximation.

Representations of Inhomogeneous $SU(n)$ Groups with Mixture of Homogeneous and Inhomogeneous Operators Diagonal*

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Explicit representations of some inhomogeneous compact $SU(n)$ groups and their algebras are constructed with certain mixtures of diagonal homogeneous and inhomogeneous operators.

I. INTRODUCTION

WHILE the subject of representations of the inhomogeneous Lorentz group has often been discussed, it is usually done with all the translation operators diagonal. An exception is the work of Lomont and Moses[1] in which only one translation operator, the energy, is diagonal as are operators (such as J_z and J^2) belonging to the homogeneous group. Further, the work on inhomogeneous groups seems to be generally confined to the inhomogeneous Lorentz group and its subgroups.

We should like to investigate here representations of inhomogeneous $SU(n)$ groups and their algebras when some members of the inhomogeneous part of the group (the Abelian invariant subgroup) and some members of the homogeneous part (the semisimple group) are simultaneously diagonal. Specifically, we consider a compact $SU(n)$ group with an Abelian group transforming as the defining representation of the homogeneous group. The semidirect product of these two groups is our inhomogeneous group. The members of the homogeneous group that are diagonal are so chosen that each, with two other operators, form the group $SU(2)$ and all the $SU(2)$ subgroups commute. This is discussed in more detail below. We now wish to construct explicit representations of these inhomogeneous groups and their algebras.

A difficulty is that the "eigenvectors" of the Abelian operators do not belong to a Hilbert space, since they are non-normalizable. A way out is to use a "rigged Hilbert space."[2] Instead of referring to treatments of such a space, we state explicitly the space containing the basis functions and its properties.

In Sec. II we specify that space, and in Sec. III we list the matrix elements of the operators between basis vectors for which the inhomogeneous operators are diagonal. In Secs. IV and V we give the representations of the inhomogeneous groups, for one homogeneous and more than one homogeneous operator diagonal, respectively. In Sec. VI the question of products of realizations and of little groups is discussed. An Appendix lists the commutation relations for the algebra A_k used in this paper.

II. THE SPACE ON WHICH THE OPERATORS ACT

The space of definition of the operators of the algebra (or group, as the case may be) need not be completely defined here. It is sufficient to state the following properties. Its subspaces include a Hilbert space (say of L^2 functions) including functions which fall off sufficiently fast[3] at infinity (rapidly decreasing functions). It also includes all exponentials, their products with constants, and members of the aforementioned Hilbert space, and sums of such terms.

In this space, we define a scalar product in the usual way, with the usual properties of a scalar product in Hilbert space, except that it is defined not for all members of the space, but only for members of the Hilbert subspace. It is for this reason that the scalar product has a finite value, which would not be true if it were defined to include the exponentials.

Considering now a functional of the rapidly decreasing functions, $T(g)$, we define the operator A acting on it as $AT(g) = T(Ag)$. An eigenfunctional

* Work supported by a grant from Long Island University.

[1] J. S. Lomont and H. E. Moses, J. Math. Phys. 5, 294, 1438 (1964).

[2] A. Bohm, International Centre for Theoretical Physics Report No. ICTP 64/9 (unpublished). I. M. Gel'fand and N. Y. Vilenkin, *Generalized Functions* (Academic Press Inc., New York, 1964), Vol. 4.

[3] We do not specify what "sufficiently fast" means as we are not investigating what conditions are necessary for a function to belong to this class, so we need not state how large a class this can be. It is sufficient for the function and its derivatives of all order to be everywhere continuous and go to zero at infinity faster than any power of the argument (or be zero outside a bounded region.) These functions are known in the theory of distributions (generalized functions) as "test functions." See for example, M. J. Lighthill, *Introduction to Fourier Analysis and Generalized Functions* (Cambridge University Press, London, 1958), p. 13; I. M. Gel'fand and G. E. Shilov, *Generalized Functions* (Academic Press Inc., New York, 1964), Vol. I, p. 2.

of the operator A is a functional which, for all members of the set of rapidly decreasing functions, satisfies $AT(g) = T(Ag) = kT(g)$, where k is some constant, the eigenvalue.

For example, consider the operators; A = operator which changes x to $x + a$, and $B = d/dx$. Their eigenfunctionals are

$$S_k(g) = \int g(x)\, dx \exp(ikx),$$

so that

$$AS_k(g) = \exp(-ika)S_k(g),$$
$$BS_k(g) = -ikS_k(g).$$

A and B are the translation and the momentum operators and are denoted as $T_i(a)$ and p_i, with the subscript giving the particular component.

III. REALIZATION OF THE OPERATORS

The realization of operators of a Lie algebra by differential forms is well known. What we wish to do here is to write matrix elements for the corresponding operators in the space we are working with.

The basis vectors are eigenfunctionals of the momentum operators of the form

$$S_k(f) = \int e^{ikx} f(x)\, dx, \tag{1}$$

where f is any rapidly decreasing function. The matrix elements $d_{k',k}$ for this set of basis vectors are defined by

$$\begin{aligned} S_{k'}(f) &= \int d_{k'k}\, S_k(f)\, dk \\ &= -\int dx\, f(x) \int dk\, d_{k'k}\, e^{ikx}. \end{aligned} \tag{2}$$

Consider now the algebra of an inhomogeneous Lie group of invariance in an n-dimensional space. Such an algebra has sums of terms of the form $J_{ij} = x_i\, d/dx_j$ for the semisimple part, and $p_k = d/dx_k$ for the inhomogeneous part. Letting $f(x_1, \cdots, x_n)$ be any rapidly decreasing function, the operators have the matrix elements for which the notation is defined by

$$J_{ij}S_k = \int d^nk'\, S_{k'}a^{ij}_{kk'}, \tag{3}$$

$$p_mS_k = \int d^nk'\, S_{k'}b^m_{kk'}, \tag{4}$$

where k and k' denote n variables. Note that ikx in the exponential is the scalar product.

It should be noted that by scalar product we mean the form of the product; that is $kx = k_ix_i$. However, this is not a scalar. The reason is that the term usually refers to a product of two vectors in the same space; here, however, we are using it to refer to vectors in different spaces, such as x space and k space. The operators of the group, or algebra, act only in x space, so that k remains unchanged or vice versa, as indicated. The term scalar product is used, even though it is not a scalar, because it has the form such that, if the vectors were in the same space, it would be a scalar.

The matrix elements can be seen to be

$$\begin{aligned} a^{ij}_{kk'} = {} & -k'_i\, \delta(k_j - k'_j)\left[\frac{d}{dk'_i}\, \delta(k_i - k'_i)\right] \\ & \times \delta(k_1 - k'_1) \cdots \delta(k_{j-1} - k'_{j-1}) \\ & \times \delta(k_{j+1} - k'_{j+1}) \cdots \delta(k_{i-1} - k'_{i-1}) \\ & \times \delta(k_{i+1} - k'_{i+1}) \cdots \delta(k_n - k'_n) \\ & + \delta_{ij}\, \delta(k_1 - k'_1) \cdots \delta(k_n - k'_n), \end{aligned} \tag{5}$$

with $\delta(k_i - k'_i)$ appearing only once, of course, for a^{ii}, and

$$\begin{aligned} b^m_{kk'} = {} & i[k'_m\, \delta(k_m - k'_m)] \\ & \times \delta(k_1 - k'_1) \cdots \delta(k_{m-1} - k'_{m-1}) \\ & \times \delta(k_{m+1} - k'_{m+1}) \cdots \delta(k_n - k'_n). \end{aligned} \tag{6}$$

Thus,

$$\begin{aligned} J_{ij}S_k(g) &= \int J_{ij}g(x)e^{ikx}\, d^nx \\ &= -\int d^nx\, g(x)J_{ij}e^{ikx} \\ &= -\int d^nx\, g(x)e^{ikx}\, \delta_{ij} \\ &= -\int d^nx\, g(x) \int d^nk'\, a^{ij}_{kk'}e^{ik'x} \\ &= -i \int d^nx\, g(x)e^{ikx}(k_ix_i) \\ &\qquad - \delta_{ij} \int d^nx\, e^{ikx}g(x) \end{aligned} \tag{7}$$

and $p_mS_k(g) = -ik_mS_k(g)$.

The commutators are

$$\begin{aligned} &(J_{ij}J_{mn} - J_{mn}J_{ij})S_k(g) \\ &\quad = -i \int d^nx\, g(x)e^{ikx}(k_nx_i\, \delta_{mj} - k_jx_m\, \delta_{ni}) \\ &\quad = (\delta_{mj}\, J_{in} - J_{mj}\, \delta_{in})S_k(g) \end{aligned} \tag{8}$$

and

$$[J_{mn}, p_t] = -\delta_{mt}\, p_n, \tag{9}$$

$$[p_t, p_s] = 0. \tag{10}$$

These, of course, are the commutation relations for the algebra A_k [the algebra of the group $SU(k+1)$] because of the choice of the operators J_{ij}. The realizations of the other series of algebras can be similarly found by taking the appropriate sums of the J_{ij}.

IV. REPRESENTATIONS WITH ONE SEMISIMPLE OPERATOR DIAGONAL

The representations of the inhomogeneous $SU(n)$ group, and its algebra, with one operator of the semisimple part and all but two of the operators of the Abelian part diagonal are now considered. The commutation relations for the algebra are given in the Appendix.

The operators that are taken as diagonal are

$$T_0 = \tfrac{1}{2}(x_1\, d/dx_1 - x_2\, d/dx_2) \tag{11}$$

and $p_t = d/dx_t$, where t is always understood to run from 3 to n. Note that p_1 and p_2, which do not commute with T_0, are not diagonal and that T_0, E_{12}, and E_{21} form the algebra A_1. We are working with the realization $E_{ij} = x_i\, d/dx_j$.

The basis functionals are

$$W_{jmk}(f) = \int f(x) x_1^{j+m} x_2^{j-m} \times \exp(ik_t x_t)\, d^n x((j+m)!\,(j-m)!)^{-\frac{1}{2}}, \tag{12}$$

where the subscript t runs from 3 to n.

We denote the matrix element of an operator A_{ij} between basis vectors W_{rsk} and $W_{r's'k'}$ as $(r's'k'|\ A_{ij}\ |rsk)$, and $\delta(k_3 - k'_3)\cdots\delta(k_n - k'_n)$ by $\delta(k-k')$. If one $\delta(k_t - k'_t)$ is listed separately, it is understood not to be included in $\delta(k-k')$.

The matrix elements of the algebra can now be calculated to give

$$(j'm'k'|\ p_t\ |jmk) = -ik_t\ \delta_{jj'}\ \delta_{mm'}\ \delta(k-k'), \tag{13}$$

$$(j'm'k'|\ p_1\ |jmk) = (j+m)^{\frac{1}{2}}\ \delta_{j',j-\frac{1}{2}}\ \delta_{m',m-\frac{1}{2}}\ \delta(k-k'), \tag{14}$$

$$(j'm'k'|\ p_2\ |jmk) = (j-m)^{\frac{1}{2}}\ \delta_{j',j-\frac{1}{2}}\ \delta_{m',m+\frac{1}{2}}\ \delta(k-k'). \tag{15}$$

It may seem surprising that the p's have matrix elements only between states j and $j - \frac{1}{2}$, whereas the product of a vector transforming as the $j = \frac{1}{2}$ representation (as the p's do) times a vector transforming as the j representation decomposes into a sum of a $j' = j - \frac{1}{2}$ representation as well as a $j' = j + \frac{1}{2}$ representation. The point is that here we are considering the p's as operators acting on the basis vectors, whereas, if we also considered terms of the form $x_1^{j+m}x_2^{j-m}p_1$ as an operator, operating on some function, then we would also have operators transforming according to the $j + \frac{1}{2}$ representation.

The remaining matrix elements are

$$(j'm'k'|\ T_0\ |jmk) = m\ \delta_{jj'}\ \delta_{mm'}\ \delta(k-k'), \tag{16}$$

$$(j'm'k'|\ E_{12}\ |jmk) = ((j+m+1)(j-m))^{\frac{1}{2}} \times \delta_{jj'}\ \delta_{m',m+1}\ \delta(k-k'), \tag{17}$$

$$(j'm'k'|\ E_{21}\ |jmk) = ((j+m)(j-m+1))^{\frac{1}{2}} \times \delta_{jj'}\ \delta_{m',m-1}\ \delta(k-k'), \tag{18}$$

$$(j'm'k'|\ H_\sigma\ |jmk) = 2j\ \delta_{jj'}\ \delta_{mm'}\ \delta(k-k') - \sum_{s=3}^{\sigma} k_s\ \delta_{jj'}\ \delta_{mm'} \left(\frac{d}{dk_s}\,\delta(k_s - k'_s)\right) \delta(k-k') + gk_\sigma\ \delta_{jj'}\ \delta_{mm'}\ (\delta(k_\sigma - k'_\sigma)/dk_\sigma)\ \delta(k-k'), \tag{19}$$

$$(j'm'k'|\ E_{1t}\ |jmk) = ik_t(j+m+1)^{\frac{1}{2}} \times \delta_{j',j+\frac{1}{2}}\ \delta_{m',m+\frac{1}{2}}\ \delta(k-k'), \tag{20}$$

$$(j'm'k'|\ E_{2t}\ |jmk) = ik_t(j-m+1)^{\frac{1}{2}} \times \delta_{j',j+\frac{1}{2}}\ \delta_{m',m-\frac{1}{2}}\ \delta(k-k'), \tag{21}$$

$$(j'm'k'|\ E_{t1}\ |jmk) = -(j+m)^{\frac{1}{2}} \times \delta_{j',j-\frac{1}{2}}\ \delta_{m',m-\frac{1}{2}}(d\ \delta(k_t - k'_t)/dk_t)\ \delta(k-k'), \tag{22}$$

$$(j'm'k'|\ E_{t2}\ |jmk) = -(j-m)^{\frac{1}{2}} \times \delta_{j',j-\frac{1}{2}}\ \delta_{m',m+\frac{1}{2}}(d\ \delta(k_t - k'_t)/dk_t)\ \delta(k-k'), \tag{23}$$

$$(j'm'k'|\ E_{tt'}\ |jmk) = -k_{t'}\ \delta_{j'j}\ \delta_{m'm}(d\ \delta(k_t - k'_t)/dk_t)\ \delta(k-k') - \delta_{tt'}\ \delta_{j'j}\ \delta_{m'm}\ \delta(k-k'). \tag{24}$$

Having given the matrix elements of the operators of the algebra, we now consider finite transformations between two variables x_i and x_j. The transformation is given by

$$\begin{aligned} x_i &= ax'_i + bx'_j, \\ x_j &= -b^*x'_i + a^*x'_j, \end{aligned} \tag{25}$$

where

$$|a|^2 + |b|^2 = 1, \tag{26}$$

and the operator inducing this transformation is denoted by $R_{ij}(a, b)$. The matrix elements for

"rotations" in the x_1x_2 plane are the well-known matrix elements for $SU(2)$ and need not be listed. The other matrix elements are

$$(i'j'k'|\, R_{t_1t_2}(a,\, b)\, |ijk)$$
$$= \delta_{j'j}\, \delta_{m'm}\, \delta(k'_{t_1} - (ak_{t_1} - b^*k_{t_2}))$$
$$\times\, \delta(k'_{t_2} - (a^*k_{t_1} + bk_{t_2}))\, \delta(k - k'). \qquad (27)$$

For a "rotation" in the x_1x_t plane (a "rotation" in the x_2x_t plane is obtained from the R_{1t} matrix element by changing the sign of m), we get

$$W_{imk} \to \frac{(ax'_1 + bx'_t)^{i+m} x_2^{i-m}}{((j+m)!\,(j-m)!)^{\frac{1}{2}}}$$
$$\times \exp\,[ik_t(a^*x'_t - b^*x'_1) + ik_sx_s]$$
$$= \sum_{\mu,n} \frac{(j+m)!\, a^{i+m-\mu} b^\mu (-ik_tb^*)^n}{(j+m-\mu)!\,\mu!\,n!\,((j+m)!\,(j-m)!)^{\frac{1}{2}}}$$
$$\times x_t'^{\mu} x_1'^{i+m-\mu+n} x_2^{i-m} \exp\,(ik_ta^*x'_t + ik_sx_s). \qquad (28)$$

So,

$$(j'm'k'|\, R_{1t}\, |jmk) = \sum_{\mu,n=0}^{n=\infty} (-i)^{\mu+n} a^{i+m-\mu} b^\mu b^{*n} k_t^n$$
$$\times \frac{((j+m)!\,(j+m+n-\mu)!)^{\frac{1}{2}}}{(j+m-\mu)!\,\mu!\,n!}\, \delta_{j',\,i+\frac{1}{2}(n-\mu)}$$
$$\times\, \delta_{m',\,m+\frac{1}{2}(n-\mu)} \left(\frac{d^\mu}{dk_t'^{\mu}}\, \delta(k'_t - a^*k_t)\right) \delta(k - k'). \qquad (29)$$

V. REPRESENTATIONS WITH SEVERAL SEMISIMPLE OPERATORS DIAGONAL

Here, we consider representations with more than one semisimple operator diagonal. Specifically, if the operators $H_{m-1} - H_m$ and $H_{n-1} - H_n$ are diagonal, then $m - n$ is required to be equal to or greater than 2. If this is the case then the operators

$$\frac{1}{2m}\,(-H_{m-1} + H_m),\, E_{m+1,m},\, E_{m,m+1}, \qquad (30)$$

and

$$\frac{1}{2n}\,(-H_{n-1} + H_n),\, E_{n+1,n},\, E_{n,n+1}, \qquad (31)$$

form algebras A_1 whose members mutually commute. It is the last phrase which is important and results from the restriction on the difference of m and n. Assuming that there are no diagonal homogeneous operators with subscripts between m and n and that r is the largest subscript on a diagonal homogeneous operator, then, with t equal to or greater than $r + 1$, we take the operators p_t, as well as $p_{m+2}, \cdots, p_{n-1}$, as diagonal for all m, n, where n is greater than m.

The basis vectors are of the form

$$\cdots \frac{x_m^{j_m+m_m} x_{m+1}^{j_m-m_m}}{((j_m+m_m)!\,(j_m-m_m)!)^{\frac{1}{2}}} \cdots$$
$$\times \frac{x_n^{j_n+m_n} x_{n+1}^{j_n-m_n}}{((j_n+m_n)!\,(j_n-m_n)!)^{\frac{1}{2}}}$$
$$\times \exp\,(ik_{m+2}x_{m+2} + \cdots + ik_tX_t). \qquad (32)$$

All the results of the last section for the matrix elements hold with the requirement that the appropriate δ's be inserted to indicate that an index does not change if the operator does not operate on the coordinate having it. These insertions are obvious and need not be written down explicitly.

There is one new set of matrix elements

$$(j'_mj'_nm'_mm'_nk'|\, E_{mn}\, |j_mj_nm_mm_nk)$$
$$= ((j_m + m_m + 1)(j_n + m_n))^{\frac{1}{2}}\, \delta_{j_m',\,j_m+\frac{1}{2}}\, \delta_{j_n',\,j_n-\frac{1}{2}}$$
$$\times\, \delta_{m_m',\,m_m+\frac{1}{2}}\, \delta_{m_n',\,m_n-\frac{1}{2}}\, \delta(k - k'). \qquad (33)$$

The matrix elements for $E_{m,n+1}$, $E_{m+1,n}$, and $E_{m+1,n+1}$ can be obtained from the above by changing the sign of the appropriate m.

Likewise, for a finite transformation between two x's, the matrix elements for any operator can be obtained from one, by the change of sign of the appropriate m, which we take as R_{mn} and use Eq. (25) with m now written for i and n for j. Then

$$(j'_mj'_nm'_mk'|\, R_{mn}(a,\, b)\, |j_mj_nm_mm_nk)$$
$$= \sum_{\mu,\nu} ((j_m + m_m + \nu - \mu)!$$
$$\times (j_n + m_m)!\,(j_n + m_n + \mu - \nu)!\,(j_n + m_n)!)^{\frac{1}{2}}$$
$$\times ((j_m + m_m - \mu)!\,\mu!\,(j_n + m_n - \nu)!\,\nu!)^{-1}$$
$$\times a^{j_m+m_m-\mu} b^\mu (-b^*)^\nu (a^*)^{j_n+m_n-\nu}$$
$$\times\, \delta_{j_m',\,j_m+\frac{1}{2}(\nu-\mu)}\, \delta_{m_m',\,m_m+\frac{1}{2}(\nu-\mu)}$$
$$\times\, \delta_{j_n',\,j_n+\frac{1}{2}(\mu-\nu)}\, \delta_{m_n',\,m_n+\frac{1}{2}(\mu-\nu)}\, \delta(k - k'). \qquad (34)$$

VI. PRODUCT OF REALIZATIONS

It is of interest to consider basis vectors of the form $T\, f(x)$, where T is a tensor (or spinor if multivalued representations are being considered) and not a function of x, while the basis vectors f are functions of x. The matrix of a transformation consisting of an element R from the homogeneous part, and an element A from the inhomogeneous part of the group can be written

$$D(R,\, A) = U(R)W(R,\, A), \qquad (35)$$

where U operates on T and W on f. Note that T is a scalar under the transformation A. For the

algebra, the differential operator corresponding to D equals the sum of differential operators corresponding to U and differential operators corresponding to W.

In the case in which all the inhomogeneous operators are diagonal, $f(x)$ is of the form of an exponential and the basis vectors T (and the operators U acting on them) are found by considering the little group.[4] We now wish to show that this method still works even when not all of the inhomogeneous operators are diagonal. The proof is almost exactly as given in Hamermesh,[4] but it seems worthwhile to give it explicitly with the few changes of wording required.

Consider any one of the inhomogeneous operators, say p_0, and all homogeneous operators G_i which commute with p_0. Clearly the G's form a group, the "little group."

Notice that we discuss this in terms of the operators p, rather than their representatives k, and that we do not need the scalar product k^2.

For an irreducible representation of the "little group," we have

$$U(G)T^0_\tau = T^0_s U(G)_{s\tau}. \tag{36}$$

Since the p's form an irreducible representation of the homogeneous group (here the defining representation has been considered), we can always find, for any p, an R belonging to the homogeneous part such that $Rp_0 = p$, and any other R' which carries p_0 to p can be written in the form $R' = RG$.

We have from Eq. (36) the irreducible representations for the subgroup made up of the G's. Corresponding to the basis functions for the G's we can now define the basis functions for the set of operators R' which take p_0 to p',

$$T^{p'}_\tau = U(R')T^0_\tau. \tag{37}$$

The rest of the proof is identical to that given in Hamermesh[4] and we get

$$U(R)T^p_\tau = T^{Rp}_s U(G)_{s\tau}. \tag{38}$$

This gives the T's and the matrices of the operators of the homogeneous group acting on them. They are scalars with respect to the p's. The matrices acting on the f's have been found in the previous sections, and so the representation is determined.

It should be noted that the "little group" here is the subgroup of transformations in a hyperplane in the space of the vectors of the defining representation of the group. The only purpose of the vector which is kept fixed is to define the hyperplane, to which it is perpendicular. Therefore, the theorem that the "little group" can be used to find the representations is a statement about the properties of a semisimple group, not about the properties of an inhomogeneous group, although it is usually stated so as to refer to the latter.

[4] M. Hamermesh, *Group Theory* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1962), Sec. 12. 7.

APPENDIX

While the algebra A_l [the algebra of $SU(l+1)$] has been extensively discussed, the canonical form of its commutation relations does not seem to be readily available. We therefore list our notation for it here. Following Racah[5] we write the commutation relations for the algebra of the general linear group as (all indices are from 1 to $l+1$);

$$[x_{ik}, x_{mn}] = \delta_{km}x_{in} - \delta_{in}x_{mk}. \tag{A1}$$

This group is not semisimple, so we define

$$x'_{ii} = x_{ii} - \frac{1}{l+1}\sum_{j=1}^{l} x_{jj}, \tag{A2}$$

which does not affect the commutation relations. We set

$$x'_{ii} = h_i \qquad \text{and} \qquad x_{ik} = E_{ik}, \tag{A3}$$

where the E's are the step operators, and the h's are the mutually commuting operators. There are $(l+1)$ of the latter but they are subjected to the condition

$$\sum_{1}^{l+1} h_i = 0. \tag{A4}$$

Thus this system is not in canonical form.[6]

To bring it into the required form, we define a new set of mutually commuting operators H_i(l in number);

$$\begin{aligned}
h_1 &= \frac{1}{2}H_1 + \frac{1}{6}H_2 + \cdots + \frac{1}{k(k+1)} \\
&\qquad \times H_k + \cdots + \frac{1}{l(l+1)}H_l, \\
&\vdots \\
h_j &= \frac{-1}{j}H_{j-1} + \frac{1}{j(j+1)}H_j + \cdots + \frac{1}{k(k+1)} \\
&\qquad \times H_k + \cdots + \frac{1}{l(l+1)}H_l, \\
h_{l+1} &= -\frac{1}{l+1}H_l,
\end{aligned} \tag{A5}$$

[5] G. Racah, "Group Theory and Spectroscopy" (Institute for Advanced Study, Lecture Notes, Princeton, New Jersey, 1951), p. 29. (unpublished).

[6] Reference 5, p. 20, Eq. (50).

which are seen to obey Eq. (A4). Solving, we get explicitly

$$\begin{aligned} H_1 &= h_1 - h_2, \\ &\vdots \\ H_j &= \sum_{i=1}^{j} h_i - (j)h_{j+1}. \end{aligned} \tag{A6}$$

The commutation relations are now (for $n > m$)

$$[H_j, E_{mn}] = \Big(\sum_{i=1}^{j} (\delta_{mi} - \delta_{ni}) - j(\delta_{m,j+1} - \delta_{n,j+1})\Big)E_{mn}, \tag{A7}$$

$$\begin{aligned} [E_{mn}, E_{nm}] &= h_m - h_n \\ &= -\frac{1}{m} H_{m-1} \\ &\quad + \sum_{k=m}^{n-2} \frac{1}{k(k+1)} H_k + \frac{1}{n-1} H_{n-1}, \end{aligned} \tag{A8}$$

$$[E_{ik}, E_{mn}] = \delta_{km}E_{in} - \delta_{in}E_{mk}. \tag{A9}$$

The roots are

$$\begin{aligned} \mathbf{r}_{1n} &= (1, 1, \cdots, 1, n, 0, 0, \cdots), \\ \mathbf{r}_{12} &= (1, 0, 0, \cdots), \\ \mathbf{r}_{kn} &= (0, 0, \cdots, -(k-1), 1, 1, \cdots, n, 0, \cdots) \\ &\qquad (n > k), \end{aligned} \tag{A10, A11}$$

where the first nonzero value occurs in the $k - 1$ column and the last in the $n - 1$ column. From this it can be seen that the right H's appear in Eq. (A8). Equation (A9) implies that

$$\mathbf{r}_{ik} + \mathbf{r}_{mn} = \mathbf{r}_{in}(\text{if } k = m) \quad \text{or} \quad \mathbf{r}_{mk}(\text{if } i = n) \tag{A12}$$

and that the equations do not hold if the conditions in parentheses do not hold. Thus, the commutation relations given by Eqs. (A7)–(A9) are in the correct canonical form. If it is desired to normalize the roots so that

$$\sum_{\alpha} \mathbf{r}_i(\alpha)\mathbf{r}_j(\alpha) = \delta_{ij}, \tag{A13}$$

then the commuting operators can be normalized to become

$$\begin{aligned} H_1' &= \{\sqrt{2}[2(l-1)+1]\}^{-1}H_1 \\ H_m' &= \{\sqrt{2}((m^2+m)(l-m) + m(m+1)^2)\}^{-1}H_m. \end{aligned} \tag{A14}$$

To find the operators of the inhomogeneous group, we consider, for the operators, the realization

$$x_{ij} = y_i\, d/dy_j, \qquad q_i = d/dy_i, \tag{A15}$$

where the q's are the inhomogeneous operators. The commutation relations are then

$$[y_i, q_k] = -\delta_{ik}, \qquad [q_i, q_k] = 0, \tag{A16}$$

$$[x_{ik}, q_j] = -\delta_{ij}q_k, \tag{A17}$$

$$[x'_{ik}, q_j] = -\delta_{ij}q_k + \frac{1}{l+1} q_j\, \delta_{ik}, \tag{A18}$$

$$[H_j, q_k] = -\sum_{i=1}^{j} \delta_{ik}q_k. \tag{A19}$$

General Coupling Coefficients for the Group $SU(3)$*

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A Hilbert space method, previously applied to the group $SU(2)$, is employed to examine the representations $\mathfrak{D}^{\lambda\mu}$ and the reduction of the direct-product representation of the group $SU(3)$. The base vectors $|\lambda\mu;\alpha>$, an orthogonal Hilbert space of homogeneous polynomials, are transformed to the base vectors $|\lambda\mu;\alpha>_c$, and are associated with the complex conjugate representation by an explicit R- conjugation operation. For the general direct-product representation $\mathfrak{D}^{\lambda_1\mu_1} \otimes \mathfrak{D}^{\lambda_2\mu_2}$, explicit expressions are derived for the vector coupling coefficients and the number of times the irreducible representation $\mathfrak{D}^{\lambda_3\mu_3}$ is contained in the direct product. Two methods of labeling the degenerate states are given, the reduction of the direct product is shown to be complete, and the symmetry relations of the $3(\lambda\mu)$ coefficients are discussed.

INTRODUCTION

THE purpose of this paper is to examine the representations $\mathfrak{D}^{\lambda\mu}$ and the reduction of the direct-product representation $\mathfrak{D}^{\lambda_1\mu_1} \otimes \mathfrak{D}^{\lambda_2\mu_2}$ in a concise, transparent manner. The particular approach is a Hilbert space method devised by Bargmann[1] to study the representations of the rotation group.

The essential ideas of the Bargmann method, the use of homogeneous polynomials of complex variables as the base vectors associated with irreducible representations, and the construction of an invariant that yields the coefficients which reduce the direct product, were employed by van der Waerden[2] in 1932, and known to Weyl[3] (1925). Bargmann's essential contribution was to combine these ideas, with his function space $\mathfrak{F}_n$,[4] in a clear and simple treatment of the many (seemingly diverse) properties of $SU(2)$. Moreover, the essential features of the method are in a form which may be generalized to $SU(3)$. The Bargmann method may also be generalized to $SU(n)$, and this problem is to be discussed in a subsequent paper.

The essential properties of the function space $\mathfrak{F}_n$ necessary to read the article have been included in Sec. 1. For a comprehensive treatment, with proofs, consult Bargmann's two papers.[1,4] The particular subspace $\mathfrak{Q}_{\lambda\mu}$ of $\mathfrak{F}_0$, the space of base vectors $|\lambda\mu;\ \alpha\rangle$, is defined in Sec. 2. The invariant Hilbert space $\mathfrak{Q}_{\lambda\mu}$ is now associated with a 2-rowed Young tableau, necessitating an antisymmetry operation with respect to the columns of the tableau. The row labels $\alpha \equiv (y,\ t,\ t_0)$ of the representations $\mathfrak{D}^{\lambda\mu}$ are defined in the standard manner using the two linear commuting operators Y, T_0, of the rank-two group, and the Casimir operator $\mathbf{T}^2$ of the $SU(2)$ subgroup. The base vectors $|\lambda\mu;\ \alpha\rangle_c$ associated with the complex conjugate representation are obtained from $|\lambda\mu;\ \alpha\rangle$ by an explicit change of variables. Section 3 is devoted to the reduction of the direct-product representation and the $3(\lambda\mu)$ symbols. Unlike the $SU(2)$ case, the condition that the invariant $h_k(k_i)$ lies in the triple-product space does not uniquely determine the parameters k_i. This is the degeneracy (or multiplicity) problem; there exists g direct-product vectors $|\lambda_3\mu_3;\ \alpha_3\rangle_k$, $k = 0,\ 1,\ \cdots,\ g-1$, associated with the irreducible representation $\mathfrak{D}^{\lambda_3\mu_3}$ contained in the representation $\mathfrak{D}^{\lambda_1\mu_1} \otimes \mathfrak{D}^{\lambda_2\mu_2}$, and Sec. 3C discusses two methods of handling this problem. The recoupling or $6(\lambda\mu)$ coefficients are discussed in an accompanying article.[5]

The notation follows, as closely as possible, that of Bargmann's article. In particular, the Hermitian adjoint of an operator, or matrix, B, is indicated by B^*, the transpose of a matrix B by ${}^tB$, and the complex conjugate of α by $\bar{\alpha}$.

1. THE HILBERT SPACE $\mathfrak{F}_n$

A. Definition of $\mathfrak{F}_n$

The elements of $\mathfrak{F}_n$ are entire analytic functions of $f(z)$, where $z = (z_1,\ z_2,\ \cdots,\ z_n)$ is a point of the

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[1] V. Bargmann, Rev. Mod. Phys. **34**, 829 (1962).

[2] B. L. van der Waerden, *Die gruppentheoretische Methode in der Quantenmechanik* (Julius Springer-Verlag, Berlin, 1932).

[3] H. Weyl, Math. Z. **23**, 271 (1925); **24**, 377 (1926); and **24** 789 (1926). The author thanks the referee for bringing this reference to his attention.

[4] For the initial development of the function space, see V. Bargmann, Commun. Pure Appl. Math. **14**, 187 (1961).

[5] M. Resnikoff, following paper, J. Math. Phys. **8**, 79 (1967).

n-dimensional complex Euclidean space C_n. For two elements f, f' of $\mathfrak{F}_n$, the inner product (f, f') is defined

$$(f, f') = \int \overline{f(z)} f'(z)\, d\mu_n(z), \tag{1.1a}$$

where $\overline{f(z)}$ is the complex conjugate of $f(z)$ and the measure $d\mu_n(z)$ is

$$d\mu_n(z) = \pi^{-n} \exp(-z\cdot\bar{z})\, d^n z, \tag{1.1b}$$

$z\cdot\bar{z} = z_1\bar{z}_1 + \cdots + z_n\bar{z}_n$, and

$$d^n z = \prod_{k=1}^{n} dx_k\, dy_k, \qquad z_k = x_k + iy_k.$$

The integral (1.1a) is taken over the whole space C_n. It may be shown that[1]

$$((z_i)^{h_i}, (z_j)^{h_j}) = \delta_{ij}\, \delta_{h_i,h_j}\, (h_i)!. \tag{1.2}$$

The operators on $\mathfrak{F}_n$ may be constructed as functions of z_n and the differential operator, $d_k \equiv \partial/\partial z_k$. The commutation relations

$$[z_k, z_m] = [d_k, d_m] = 0, \qquad [d_k, z_m] = \delta_{km} \tag{1.3}$$

are obvious. For any elements f, g of $\mathfrak{F}_n$, z_k and d_k are adjoint with respect to the inner product

$$(z_k f, g) = (f, d_k g), \tag{1.4}$$

as may be shown by expanding $f(z)$ in a power series (see Bargmann[1]).

B. Bargmann Operators M_{ij}

On the Hilbert space $\mathfrak{F}_3$, define the differential operators M_{ij}

$$M_{ij} f(\zeta) = \tfrac{1}{2} \sum_{\alpha,\beta=1}^{3} \zeta_\alpha (m_{ij})_{\alpha\beta} (\partial/\partial\zeta_\beta) f(\zeta), \tag{1.5}$$

where $\zeta = (\xi, \eta, \sigma)$ replaces $z = (z_1, z_2, z_3)$ as a point in the space C_3, and the matrices m_{ij} are linear combinations of the infinitesimal matrices b_j,

$$ib_j = (\partial/\partial\theta_j) T_u f\,|_{\theta_k=0} \text{ all } k, \quad j = 1, \cdots, 8, \tag{1.6}$$

θ_k, $k = 1, \cdots, 8$, representing the eight parameters of the group.[6] The matrices m_{ij} differ by factors from the infinitesimal matrices of Behrends *et al.*[7]:

$$\tfrac{1}{2}(m_{12}) = 6^{\frac{1}{2}} E_1, \qquad \tfrac{1}{2}(m_{21}) = 6^{\frac{1}{2}} E_{-1},$$
$$\tfrac{1}{2}(m_{13}) = 6^{\frac{1}{2}} E_2, \qquad \tfrac{1}{2}(m_{31}) = 6^{\frac{1}{2}} E_{-2},$$
$$\tfrac{1}{2}(m_{23}) = 6^{\frac{1}{2}} E_3, \qquad \tfrac{1}{2}(m_{32}) = 6^{\frac{1}{2}} E_{-3},$$
$$\tfrac{1}{2}(t_0) = \sqrt{3} H_1, \qquad \tfrac{1}{2}(y) = 6 H_2,$$

y, t_0 being the two linear commuting matrices of the rank-two group.

The Bargmann differential operators, Eq. (1.5), are

$$M_{12} = \xi \frac{\partial}{\partial\eta}, \quad M_{21} = \eta \frac{\partial}{\partial\xi}, \quad M_{13} = \xi \frac{\partial}{\partial\sigma},$$
$$M_{31} = \sigma \frac{\partial}{\partial\xi}, \quad M_{23} = \eta \frac{\partial}{\partial\sigma}, \quad M_{32} = \sigma \frac{\partial}{\partial\eta},$$
$$T_0 = \frac{1}{2}\left(\xi \frac{\partial}{\partial\xi} - \eta \frac{\partial}{\partial\eta}\right), \quad Y = \xi \frac{\partial}{\partial\xi} + \eta \frac{\partial}{\partial\eta} - 2\sigma \frac{\partial}{\partial\sigma}. \tag{1.7}$$

If $f(\zeta)$ is a homogeneous polynomial of degree m in ζ, then so is $M_{ij} f(\zeta)$, according to the definition Eq. (1.5). Since the invariant Hilbert space of base vectors is given by the degree in the variables ζ, and since the function $M_{ij} f$ has the same degree m, the operators M_{ij} are said to operate *within* the Hilbert space, as raising and lowering operators.

Note that, using Eq. (1.4),

$$(M_{ij} f, g) = (f, M_{ji} g). \tag{1.8}$$

In particular, Y, T_0 are Hermitian with respect to the inner product.

2. THE REPRESENTATIONS $\mathfrak{D}^{\lambda\mu}$

A. Hilbert Space $\mathfrak{Q}_{\lambda\mu}$

Let an element f of the function space $\mathfrak{F}_6$ be written $f(\zeta_1, \zeta_2)$, where ζ_1, ζ_2 are points in a three-dimensional complex Euclidean space C_3. $\mathfrak{Q}_{\lambda\mu}$, the subspace of $\mathfrak{F}_6$, is the space of homogeneous polynomials $f(\zeta_1, \zeta_2)$ of degree $\lambda + \mu$ in ζ_1, and μ in ζ_2.

To put this in operator form, define the operator[8] T_{ij}

$$T_{ij} = \xi_i \frac{\partial}{\partial\xi_j} + \eta_i \frac{\partial}{\partial\eta_j} + \sigma_i \frac{\partial}{\partial\sigma_j}. \tag{2.1}$$

An element $f(\zeta_1, \zeta_2)$ belongs to $\mathfrak{Q}_{\lambda\mu}$ if and only if the Euler equations

$$T_{11} f = (\lambda + \mu) f, \qquad T_{22} f = \mu f \tag{2.2}$$

are satisfied.[9]

The spaces $\mathfrak{Q}_{\lambda\mu}$ and $\mathfrak{Q}_{\lambda'\mu'}$ are obviously orthogonal for $\lambda \neq \lambda'$, or $\mu \neq \mu'$, by Eq. (1.2). The function space $\mathfrak{F}_6$ may then be decomposed into the sum of mutually orthogonal subspaces

$$\mathfrak{F}_6 = \sum_{\lambda,\mu} \mathfrak{Q}_{\lambda\mu}. \tag{2.3}$$

[6] The matrices b_j and m_{ij} may, of course, be obtained directly from the $SU(3)$ matrix as parameterized by F. D. Murnaghan, *The Unitary and Rotation Groups* (Spartan Books, Washington, D. C., 1962), in analogy to the $SU(2)$ case. See M. Resnikoff, University of Michigan preprint (1965).

[7] R. E. Behrends, J. Dreitlein, C. Fronsdal, and B. W. Lee, Rev. Mod. Phys. **34**, 1 (1962).

[8] The operator T_{ij} was first considered by V. Bargmann and M. Moshinsky, Nucl. Phys. **18**, 697 (1960); **23**, 177 (1961).

[9] T_{11} and T_{22} are analogous to Bargmann's operator N, $N\cdot v^i_m = j\cdot v^i_m$ (see Ref. 1).

The Euler equations (2.2) require that the homogeneous polynomials $f(\zeta_1, \zeta_2)$ be of degree $\lambda + \mu$ in ζ_1, and degree μ in ζ_2, the number of boxes in the first and second rows, respectively, of the Young tableau for $SU(3)$. The additional condition from the Young tableau is that $f(\zeta_1, \zeta_2)$ be antisymmetric in the μ columns. Since ζ_2 is of degree μ, ζ_2 may occur only in the antisymmetric forms

$$\begin{aligned}\delta_{12} &= (\delta_{12}^{(1)}, \delta_{12}^{(2)}, \delta_{12}^{(3)}) \\ &= (\eta_1\sigma_2 - \eta_2\sigma_1, \sigma_1\xi_2 - \sigma_2\xi_1, \xi_1\eta_2 - \xi_2\eta_1).\end{aligned} \tag{2.4}$$

That is, the homogeneous polynomials f must have the functional form $f(\zeta_1, \delta_{12})$.[10] The differential form of this antisymmetry requirement is that

$$T_{12}f(\zeta_1, \zeta_2) = 0, \tag{2.5}$$

where T_{ij} is given by Eq. (2.1). T_{12} serves as the Weyl alternation operator,[11] $\Sigma\delta_q \cdot \mathbf{g}$, the operator which antisymmetrizes an unsymmetrized tensor with respect to the columns of a Young tableau.

The unitary transformations T_U on $\mathfrak{F}_6$ may be defined

$$T_U f(\zeta_1, \zeta_2) = f({}^tU\zeta_1, {}^tU\zeta_2), \tag{2.6}$$

where ${}^tU$ is the transpose of U, an element of $SU(3)$. When the variables ζ_1, ζ_2 in C_3 undergo a unitary transformation U, T_U defines a transformation of the elements $f(\zeta_1, \zeta_2)$ in the Hermitian space $\mathfrak{F}_6$. It may be shown that the transformations T_U form a unitary representation.[1] The spaces $\mathfrak{Q}_{\lambda\mu}$ are obviously invariant under a unitary transformation T_U, since the right side of Eq. (2.6) may again be expressed as a linear combination of polynomials $f(\zeta_1, \zeta_2)$ of the same degree in ζ_1, ζ_2.

For $\mathfrak{F}_6$, the Bargmann differential operators [Eqs. (1.5) and (1.7)] become

$$M_{ij}(\zeta_1, \zeta_2) = M_{ij}(\zeta_1) + M_{ij}(\zeta_2) \tag{2.7}$$

from Eq. (2.6).

B. Row Labels α

The row labels α of the representations $\mathfrak{D}^{\lambda\mu}$ are specified in the usual manner by the two linear commuting operators Y, T_0 of the rank-two group, and

$$\mathbf{T}^2 = T_0^2 + T_0 + M_{21}M_{12}, \tag{2.8}$$

the Casimir operator of the subgroup $SU(2)$. The base vector is uniquely specified by the conditions (2.2), (2.5), and

$$\begin{aligned} Y\,|\lambda\mu;\alpha\rangle &= y\,|\lambda\mu;\alpha\rangle, \\ T_0\,|\lambda\mu;\alpha\rangle &= t_0\,|\lambda\mu;\alpha\rangle, \\ \mathbf{T}^2\,|\lambda\mu;\alpha\rangle &= t(t+1)\,|\lambda\mu;\alpha\rangle, \end{aligned}$$

where $\alpha \equiv (y, t, t_0)$. The numbers t and t_0 are the isospin and the z component of the isospin, whereas y is 3 times the hypercharge quantum number. Since the operators (2.2), and $\mathbf{T}^2$, T_0, Y are Hermitian with respect to the inner product, the base vectors are orthogonal,

$$(|\lambda\mu;\alpha\rangle, |\lambda'\mu';\alpha'\rangle) = \delta_{\lambda\lambda'}\,\delta_{\mu\mu'}\,\delta_{\alpha\alpha'} \tag{2.9}$$

using Eq. (1.2).

The base vector $|\lambda\mu;\alpha\rangle$, as an explicit function of ζ_1, ζ_2, may be constructed with the appropriate raising and lowering operators of $SU(3)$ using the operators M_{ij} and appropriate products. The method has been used by Elliott,[12] Elliott and Harvey,[13] Hecht,[14] and Gel'fand and Zeitlin,[15] and the base vectors appear in the literature (see Bargmann and Moshinsky,[8] Moshinsky,[16] Baird and Biedenharn,[17] and Mukunda and Pandit[18]). Only the result is quoted here.

$$\begin{aligned} |\lambda\mu;\alpha> &= N(\lambda\mu;\alpha)(-1)^q \\ &\times \sum_k \binom{r}{k} \frac{(\mu-q)!\,p!}{(\mu-q-k)!\,[p-(r-k)]!} \\ &\times \xi_1^{p-(r-k)}\eta_1^{r-k}\sigma_1^{\lambda-p}(\delta_{12}^{(1)})^k(-\delta_{12}^{(2)})^{\mu-q-k}(\delta_{12}^{(3)})^q, \end{aligned} \tag{2.10a}$$

where $N(\lambda\mu;\alpha)$ normalizes $|\lambda\mu;\alpha\rangle$ to unity (derived in Appendix A),

$$\begin{aligned} &N(\lambda\mu;\alpha) \\ &= \left\{\frac{(\lambda+1)!\,(\mu+p-q+1)!}{p!\,q!\,(\mu-q)!\,(\lambda-p)!\,(\mu+p+1)!\,(\lambda+\mu-q+1)!}\right. \\ &\quad \left.\times \frac{(2t-r)!}{(2t)!\,r!}\right\}^{\frac{1}{2}} \end{aligned} \tag{2.10b}$$

and

$$\begin{aligned} y &= -(2\lambda+\mu) + 3(p+q), && 0 \le p \le \lambda, \\ t &= \tfrac{1}{2}\mu + \tfrac{1}{2}(p-q), && 0 \le q \le \mu, \\ t_0 &= t - r, && r = 0, 1, \cdots, 2t. \end{aligned} \tag{2.10c}$$

[10] $f(\zeta_1,\zeta_2)$ and $f(\zeta_1,\delta_{12})$ are used interchangeably in the article.

[11] H. Weyl, *The Theory of Groups and Quantum Mechanics* (Dover Publications, Inc., New York, 1931), p. 359.

[12] J. P. Elliott, Proc. Roy. Soc. (London) **A245**, 128, 562 (1958).

[13] J. P. Elliott and M. Harvey, Proc. Roy. Soc. (London) **A272**, 557 (1963).

[14] K. T. Hecht, Nucl. Phys. **62**, 1 (1965).

[15] I. M. Gel'fand and M. L. Zeitlin, Doklady Akad. Nauk SSSR **71**, 825 (1950).

[16] M. Moshinsky, Nucl. Phys. **31**, 384 (1962).

[17] G. Baird and L. Biedenharn, J. Math. Phys. **4**, 1449 (1963).

[18] N. Mukunda and L. K. Pandit, J. Math Phys. **6**, 746 (1965).

The second factor in Eq. (2.10b) may be recognized as the Condon and Shortley[19] normalization for the lowering operator $T_- = M_{21}$. A specific phase convention has been assumed,

$$T_- \,|\lambda\mu; ytt_0> = C_1 \,|\lambda\mu; ytt_0 - 1>, \qquad (2.11a)$$

where C_1 is a positive constant. In addition, the requirements

$$(|\lambda\mu; y + 3, (t + \tfrac{1}{2}), (t_0 + \tfrac{1}{2})\rangle, M_{13} \,|\lambda\mu; \alpha\rangle) > 0, \qquad (2.11b)$$

$$(|\lambda\mu; y + 3, (t - \tfrac{1}{2}), (t_0 + \tfrac{1}{2})\rangle, M_{13} \,|\lambda\mu; \alpha\rangle) > 0 \qquad (2.11c)$$

specify the phase of $|\lambda\mu; \alpha\rangle$ with respect to p and q. This phase convention agrees with Elliott and Harvey,[13] and Hecht[14] (though their hypercharge is the negative of the above), but De Swart,[20] Biedenharn,[21] Kuriyan, Lurie, and Macfarlane,[22] and Mukunda and Pandit,[18] assume the matrix element [Eq. (2.11c)] to be negative, since the $SU(2)$ factor of Eq. (2.12c) is negative-definite.[23]

C. The Representations $\mathfrak{D}^{\lambda\mu}$

1. Irreducibility

T_U defines a transformation of the elements $f(z)$ in the Hermitian space $\mathfrak{H}_6$ [see Eq. (2.6)]. The unitary representations $\mathfrak{D}^{\lambda\mu}(U)$ are defined by restricting T_U to act in the subspace $\mathfrak{Q}_{\lambda\mu}$:

$$T_U \,|\lambda\mu; \alpha\rangle = \sum_{\alpha'} \mathfrak{D}^{\lambda\mu}_{\alpha'\alpha}(U) \,|\lambda\mu; \alpha'\rangle, \qquad (2.12)$$

$$\mathfrak{D}^{\lambda\mu}_{\alpha'\alpha}(U) = (|\lambda\mu; \alpha'\rangle, T_U \,|\lambda\mu; \alpha\rangle) \qquad (2.13)$$

using Eq. (2.9). The representations $\mathfrak{D}^{\lambda\mu}$ are irreducible.[24] By Schur's lemma, it is sufficient to prove that every linear operator A defined on $\mathfrak{Q}_{\lambda\mu}$ (which commutes with all T_U) is necessarily of the form $A = \alpha \cdot 1$. If A commutes with all T_U, then it must also commute with all the generators M_{ij}, by Eq. (1.6). The operators T_{11}, T_{22}, which define the invariant spaces $\mathfrak{Q}_{\lambda\mu}$, and the antisymmetry operator T_{12} (or T_{21}), commute with the generators of the group M_{ij} and are of the form $A = \alpha \cdot 1$. There are no other linear commuting operators.

2. Inequivalence

The representations $\mathfrak{D}^{\lambda\mu}(U)$ and $\mathfrak{D}^{\lambda'\mu'}(U)$ are inequivalent for $\lambda \neq \lambda'$ or $\mu \neq \mu'$. The proof follows from Schur's lemma.[25] If $e_1, \cdots, e_m$ and $f_1, \cdots, f_n$ are two sets of vectors in the spaces $\mathfrak{Q}$, $\mathfrak{Q}'$, respectively, and if V_α is a set of unitary operators defined on $\mathfrak{Q}$, $\mathfrak{Q}'$, then

$$V_\alpha e_i = \sum_{j=1}^{m} e_j \rho_{ji}(\alpha), \qquad V_\alpha f_r = \sum_{s=1}^{n} f_s \sigma_{sr}(\alpha),$$

where the matrices $\rho_{ji}(\alpha)$, $\sigma_{sr}(\alpha)$ are unitary and irreducible. Let $\beta_{ir} = (e_i, f_r)$ be the inner product matrix. Then it may be shown[1], employing matrix notation, that $\rho(\alpha)\beta = \beta\sigma(\alpha)$. That is, β is a mapping of the space $\mathfrak{D}$ onto $\mathfrak{D}'$. Schur's lemma implies either

(1) $\beta = 0$, i.e., $(e_i, f_r) = 0$, for all i, r, or

(2) the representations are equivalent and β is a multiple of the unit matrix

$$(e_i, f_r) = \beta_{ir} = \epsilon\, \delta_{ir}. \qquad (2.14)$$

Then, the dimensions of the representations are equal, and for $e_i = f_i$,

$$(e_i, e_j) = \epsilon\, \delta_{ij}. \qquad (2.15)$$

The representations are certainly inequivalent if the dimensions

$$N = \tfrac{1}{2}(\mu + 1)(\lambda + 1)(\lambda + \mu + 2)$$

of $\mathfrak{Q}_{\lambda\mu}$, $\mathfrak{Q}_{\lambda'\mu'}$ are not the same. In the cases where the dimension N is the same for different spaces[26] $\mathfrak{Q}_{\lambda\mu}$, $\mathfrak{Q}_{\lambda'\mu'}$, the inner product is zero [see Eq. (2.9)] and an equivalence transformation β cannot be found.

D. Complex Conjugate Representation $\overline{\mathfrak{D}^{\lambda\mu}(u)}$

Since the $SU(3)$ transformation matrix is unimodular, the 3×3 determinant

$$\begin{vmatrix} \xi_1 & \xi_2 & \xi_3 \\ \eta_1 & \eta_2 & \eta_3 \\ \sigma_1 & \sigma_2 & \sigma_3 \end{vmatrix} = \zeta_3 \cdot (\zeta_1 \times \zeta_2) = \zeta_3 \cdot \delta_{12} \qquad (2.16)$$

is invariant under a unitary transformation. This implies

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[19] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, England, 1935).

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

[21] L. C. Biedenharn, Phys. Letters **3**, 69 (1962).

[22] J. G. Kuriyan, D. Lurie, and A. J. Macfarlane, J. Math. Phys. **6**, 722 (1965).

[23] For the Biedenharn phase convention, the base vector Eq. (2.10) must be multiplied by the factor $(-1)^q$.

[24] A different proof of the irreducibility of the representations may be found in M. Moshinsky, J. Math. Phys. **4**, 1128 (1963).

[25] See the statement of Schur's lemma given by Bargmann in Ref. 1.

[26] The dimension is the same for $\mathfrak{Q}_{\lambda\mu}$ and $\mathfrak{Q}_{\mu\lambda}$, but there are other possibilities, e.g., for $N = 15$, the following partitions $[\lambda,\mu]$ exist: [2,1], [1,2], [4,0], [0,4].

$$\sum_{\alpha} {}^{t}U_{i\alpha}\, \mathfrak{D}'^{(0,1)}_{\alpha k}(U) = \delta_{ik}, \tag{2.17}$$

since $\mathfrak{D}^{(1,0)}(U) = U$. $\mathfrak{D}'^{(0,1)}$ is the irreducible unitary representation associated with δ_{12}. From unitarity,

$$\mathfrak{D}'^{(0,1)}(U) = \bar{U}. \tag{2.18}$$

When the variables ζ_1, ζ_2 undergo unitary transformations, the 2×2 antisymmetric forms δ_{12} transform with respect to the complex conjugate representation. Given a base vector of the functional form $f(\zeta_1, \delta_{12})$, the base vector $|\lambda\mu;\, \alpha\rangle_c$ associated with the complex conjugate representation

$$T_U\, |\lambda\mu;\, \alpha\rangle_c = \sum_{\alpha'} \overline{\mathfrak{D}^{\lambda\mu}_{\alpha',\alpha}(U)}\, |\lambda\mu;\, \alpha'\rangle_c \tag{2.19}$$

may be obtained by exchanging $\zeta_1 \leftrightarrow \delta_{12}$, and this is the explicit R-conjugation transformation.[27,28] Define the transformation R as

$$Rf(\zeta_1, \delta_{12}) = f(\delta_{12}, \zeta_1). \tag{2.20}$$

Then,

$$R\, |\lambda\mu;\, \alpha\rangle = C\, |\lambda\mu;\, \alpha\rangle_c, \tag{2.21a}$$

where

$$C = \left\{\frac{(\lambda+1)!}{(\mu+1)!}\right\}^{\frac{1}{2}}. \tag{2.21b}$$

The operation R, Eq. (2.19), is not a unitary transformation; the base vector $|\lambda\mu;\, \alpha\rangle_c$ must be normalized to unity, Eq. (2.21).

If the following changes are made in the base vector $|\lambda\mu;\, \alpha\rangle$: (a) $\lambda \leftrightarrow \mu$, $p \to \mu - q$, $q \to \lambda - p$, $r \to 2t - r$ and (b) $k \to k - p + r$, then, upon comparison with $|\lambda\mu;\, \alpha\rangle_c$, one obtains

$$|\lambda\mu;\, \alpha\rangle_c = (-1)^{y/2 - t_0}\, |\mu\lambda;\, -\alpha\rangle, \tag{2.22a}$$

where

$$-\alpha \equiv (-y,\, t,\, -t_0).^{29} \tag{2.22b}$$

The operation R is thus a one-to-one mapping of $\mathfrak{Q}_{\lambda\mu}$ onto $\mathfrak{Q}_{\mu\lambda}$.

Relation (2.22) is analogous to the $SU(2)$ result[1]

$$w^i_m = (-1)^{i+m} v^i_{-m}. \tag{2.23}$$

The important distinction between Eqs. (2.21) and (2.22) is that w^i_m was a member of the same Hilbert space as v^i_m, but $|\lambda\mu;\, \alpha\rangle_c$ is a member of $\mathfrak{Q}_{\mu\lambda}$ (not $\mathfrak{Q}_{\lambda\mu}$).

3. REDUCTION OF THE DIRECT-PRODUCT REPRESENTATION[30]

A. Reduction of $\mathfrak{D}^{\lambda_1\mu_1} \otimes \mathfrak{D}^{\lambda_2\mu_2}$

Let $\mathfrak{F}^{(1)}_6$, $\mathfrak{F}^{(2)}_6$ be the Hilbert spaces of analytic functions $f(\zeta_1, \zeta_2)$, $f(\zeta_3, \zeta_4)$, respectively, where $\zeta_i = (\xi_i, \eta_i, \sigma_i)$ is a member of C_3. $\mathfrak{F}_{12} = \mathfrak{F}^{(1)}_6 \otimes \mathfrak{F}^{(2)}_6$ is a Hilbert space of analytic functions $f(\zeta_1, \zeta_2; \zeta_3, \zeta_4)$. The subspace

$$\mathfrak{Q}_{\lambda_1\mu_1\lambda_2\mu_2} = \mathfrak{Q}_{\lambda_1\mu_1} \otimes \mathfrak{Q}_{\lambda_2\mu_2}$$

of $\mathfrak{F}_{12}$ is spanned by the N_1N_2 direct-product vectors $|\lambda_1\mu_1;\, \alpha_1\rangle \mid \lambda_2\mu_2;\, \alpha_2\rangle$, where $N_i = \frac{1}{2}(\lambda_i + 1)(\mu_i + 1)(\lambda_i + \mu_i + 2)$, $i = 1, 2, 3$, the dimension of the ith space. For any $SU(3)$ transformation U, the operators $T^{(1)}_U$ and $T^{(2)}_U$ are defined on $\mathfrak{F}^{(1)}_6$ and $\mathfrak{F}^{(2)}_6$ respectively, by Eq. (2.6). For a function $f(\zeta_1, \zeta_2; \zeta_3, \zeta_4)$, a member of $\mathfrak{F}_{12}$, $T^{(1,2)}_U$ forms a unitary representation

$$(T^{(1,2)}_U f)(\zeta_1, \zeta_2; \zeta_3, \zeta_4) = f({}^{t}U\zeta_1, {}^{t}U\zeta_2; {}^{t}U\zeta_3, {}^{t}U\zeta_4).$$

Further, since for $\mathfrak{Q}_{\lambda_1\mu_1\lambda_2\mu_2}$,

$$f(\zeta_1, \zeta_2; \zeta_3, \zeta_4) = f(\zeta_1, \zeta_2) f(\zeta_3, \zeta_4),$$

$$(T^{(1,2)}_U f)(\zeta_1, \zeta_2; \zeta_3, \zeta_4) = f({}^{t}U\zeta_1, {}^{t}U\zeta_2) f({}^{t}U\zeta_3, {}^{t}U\zeta_4)$$
$$= [(T^{(1)}_U f)(\zeta_1, \zeta_2)][(T^{(2)}_U f)(\zeta_3, \zeta_4)],$$

the result follows that

$$T^{(1,2)}_U = T^{(1)}_U \otimes T^{(2)}_U. \tag{3.1}$$

Thus, $T^{(1,2)}_U$, restricted to the space $\mathfrak{Q}_{\lambda_1\mu_1\lambda_2\mu_2}$, provides the direct-product representation

$$\mathfrak{D}^{\lambda_1\mu_1}(U) \otimes \mathfrak{D}^{\lambda_2\mu_2}(U).$$

The infinitesimal transformations on $\mathfrak{F}_{12}$ are

$$M_{ij}(\zeta_1, \zeta_2; \zeta_3, \zeta_4) = M_{ij}(\zeta_1, \zeta_2) + M_{ij}(\zeta_3, \zeta_4). \tag{3.2}$$

The extension to $\mathfrak{F}_{18}$ is obvious. Define the transformation

$$(T^{(1,2,3)}_U f)(\zeta_1, \zeta_2; \zeta_3, \zeta_4; \zeta_5, \zeta_6)$$
$$= f({}^{t}U\zeta_1, {}^{t}U\zeta_2; {}^{t}U\zeta_3, {}^{t}U\zeta_4; {}^{t}U\zeta_5, {}^{t}U\zeta_6).$$

Then,

$$T^{(1,2,3)}_U = T^{(1,2)}_U \otimes T^{(3)}_U = T^{(1)}_U \otimes T^{(2)}_U \otimes T^{(3)}_U. \tag{3.3}$$

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[27] D. Lurie and A. J. Macfarlane, J. Math. Phys. 5, 565 (1964) give an implicit derivation of R-conjugation. The term "R-conjugation" is due to M. Gell-Mann, California Institute of Technology Report CTSL-20 (1961).

[28] See also G. E. Baird and L. C. Biedenharn, J. Math. Phys. 5, 1723 (1964) for a discussion of the conjugation operation for $SU(n)$ in terms of operator mappings.

[29] Since $y = 3 \times$ hypercharge (Y),
$$(-1)^{y/2+t_0} = (-1)^{y/2-t_0+2/3(\lambda+2\mu)}$$
which agrees with de Swart (Ref. 20).

[30] The discussion of Sec. 3A follows from that given by Bargmann (Ref. 1) for the group $SU(2)$. The functional space is now $\mathfrak{F}_6$ and the proof of the theorem on the reduction of the direct product must be altered to account for the degeneracy in direct product states.

The direct product representation may be reduced according to the formula

$$[\lambda_1\mu_1] \otimes [\lambda_2\mu_2] = \sum g(\lambda_i\mu_i)[\lambda_3\mu_3], \qquad (3.4)$$

where $g(\lambda_i\mu_i)$ is the degeneracy, the number of times the irreducible representation $\mathfrak{D}^{\lambda_3\mu_3}$ is contained in $\mathfrak{D}^{\lambda_1\mu_1} \otimes \mathfrak{D}^{\lambda_2\mu_2}$. For each partition $[\lambda_3\mu_3]$ there exists gN_3 independent products $|\lambda_1\mu_1;\ \alpha_1\rangle |\lambda_2\mu_2;\ \alpha_2\rangle$. Associate the index k with the space of N_3 orthonormal base vectors[31]

$$\mathfrak{Q}^{(k)}_{\lambda_1\mu_1\lambda_3\mu_3}, \qquad k = 0, 1, \cdots, g-1.$$

If the irreducible representation $\mathfrak{D}^{\lambda_3\mu_3}$ is contained in the product representation $\mathfrak{D}^{\lambda_1\mu_1} \otimes \mathfrak{D}^{\lambda_2\mu_2}$, there exists N_3 orthonormalized product base vectors

$$|\lambda_3\mu_3;\ \alpha_3\rangle_k \quad \text{in} \quad \mathfrak{Q}^{(k)}_{\lambda_1\mu_1\lambda_2\mu_2}$$

such that

$$T_U^{(1,2)}\ |\lambda_3\mu_3;\ \alpha_3\rangle_k = \sum_{\alpha_3'} \mathfrak{D}^{\lambda_3\mu_3}_{\alpha_3',\alpha_3}(U)\ |\lambda_3\mu_3;\ \alpha_3'\rangle_k. \qquad (3.5)$$

(Note that the irreducible representation $\mathfrak{D}^{\lambda_3\mu_3}$ has no subindex k because the equivalence transformation $\beta_{kk'}$ [see Eq. (2.14)] equals $\delta_{kk'}$, since the base vectors $|\lambda_3\mu_3;\ \alpha_3\rangle_k$ are also assumed orthogonal with respect to k.) Consider the expression

$$a_k = \sum_{\alpha_3} |\lambda_3\mu_3;\ \alpha_3\rangle_k\ |\lambda_3\mu_3;\ \alpha_3\rangle_c,$$
$$k = 0, 1, \cdots, g-1 \qquad (3.6)$$

as a member of the space

$$\mathfrak{Q}^{(k)}_{\lambda_1\mu_1\lambda_2\mu_2\mu_3\lambda_3}.$$

a_k, being the sum of orthonormal functions, is not equal to zero. If $\mathfrak{D}^{\lambda_3\mu_3}(U)$ is contained in the product representation $\mathfrak{D}^{\lambda_1\mu_1} \otimes \mathfrak{D}^{\lambda_2\mu_2}$, then a_k is invariant in the triple-product space

$$\mathfrak{Q}^{(k)}_{\lambda_1\mu_1\lambda_2\mu_2\mu_3\lambda_3}:$$

$$T_U^{(1,2,3)} a_k = \sum_{\alpha_3} (T_U^{(1,2)}\ |\lambda_3\mu_3;\ \alpha_3\rangle_k)(T_U^{(3)}\ |\lambda_3\mu_3;\ \alpha_3\rangle_c),$$

from Eq. (3.3)

$$= \sum_{\alpha_3} \{\sum_{\alpha_3'} |\lambda_3\mu_3;\ \alpha_3'\rangle_k\ \mathfrak{D}^{\lambda_3\mu_3}_{\alpha_3',\alpha_3}(U)\}$$
$$\times \{\sum_{\alpha_3''} |\lambda_3\mu_3;\ \alpha_3''\rangle_c\ \overline{\mathfrak{D}^{\lambda_3\mu_3}_{\alpha_3'',\alpha_3}(U)}\},$$

using Eqs. (3.5) and (2.19)

$$= \sum_{\alpha_3',\alpha_3''} |\lambda_3\mu_3;\ \alpha_3'\rangle_k\ |\lambda_3\mu_3;\ \alpha_3''\rangle_c$$
$$\times \sum_{\alpha_3} \mathfrak{D}^{\lambda_3\mu_3}_{\alpha_3',\alpha_3}(U)\ \overline{\mathfrak{D}^{\lambda_3\mu_3}_{\alpha_3'',\alpha_3}(U)}$$
$$= \sum_{\alpha_3',\alpha_3''} |\lambda_3\mu_3;\ \alpha_3'\rangle_k\ |\lambda_3\mu_3;\ \alpha_3''\rangle_c\ \delta_{\alpha_3',\alpha_3''},$$

since the representations are unitary. Hence,

$$T_U^{(1,2,3)} a_k = a_k. \qquad (3.7)$$

Conversely, let h_k be an orthonormal function in $\mathfrak{Q}^{(k)}_{\lambda_1\mu_1\lambda_2\mu_2\mu_3\lambda_3}$ such that

$$T_U^{(1,2,3)} h_k = h_k. \qquad (3.8)$$

Since the functions $|\lambda_3\mu_3;\ \alpha_3\rangle_c$ span the space $\mathfrak{Q}_{\mu_3\lambda_3}$, h_k has an expansion

$$h_k = \sum_{\alpha_3} \chi^{(k)}_{\alpha_3}\ |\lambda_3\mu_3;\ \alpha_3\rangle_c \qquad (3.9)$$

with $\chi^{(k)}_{\alpha_3}$ uniquely determined in

$$\mathfrak{Q}^{(k)}_{\lambda_1\mu_1\lambda_2\mu_2}:$$

$$T_U^{(1,2,3)} h_k = \sum_{\alpha_3} (T_U^{(1,2)} \chi^{(k)}_{\alpha_3})(T_U^{(3)}\ |\lambda_3\mu_3;\ \alpha_3\rangle_c)$$

using Eq. (3.3).

$$= \sum_{\alpha_3'} \{\sum_{\alpha_3} (T_U^{(1,2)} \chi^{(k)}_{\alpha_3})\ \mathfrak{D}^{\lambda_3\mu_3}_{\alpha_3',\alpha_3}(U)\}\ |\lambda_3\mu_3;\ \alpha_3\rangle_c$$

by definition, Eq. (2.19).

$$= \sum_{\alpha_3''} \chi^{(k)}_{\alpha_3''}\ |\lambda_3\mu_3;\ \alpha_3''\rangle_c$$

by assumption (3.8). Thus,

$$\chi^{(k)}_{\alpha_3''} = \sum_{\alpha_3} (T_U^{(1,2)} \chi^{(k)}_{\alpha_3})\ \mathfrak{D}^{\lambda_3\mu_3}_{\alpha_3'',\alpha_3}(U). \qquad (3.10)$$

Multiply (3.10) by $\overline{\mathfrak{D}^{\lambda_3\mu_3}_{\alpha_3'',\alpha_3}(U)}$

and sum over α_3''. From the unitarity of the representations,

$$T_U^{(1,2)} \chi^{(k)}_{\alpha_3} = \sum_{\alpha_3''} \chi^{(k)}_{\alpha_3''}\ \mathfrak{D}^{\lambda_3\mu_3}_{\alpha_3'',\alpha_3}(U). \qquad (3.11)$$

Consider the inner product of h_k:

$$(h_k,\ h_{k'}) = \sum_{\alpha_3} (\chi^{(k)}_{\alpha_3}\ |\lambda_3\mu_3;\ \alpha_3\rangle_c,\ \chi^{(k')}_{\alpha_3'}\ |\lambda_3'\mu_3';\ \alpha_3'\rangle_c)$$
$$= \sum_{\alpha_3} (\chi^{(k)}_{\alpha_3},\ \chi^{(k')}_{\alpha_3}),$$

since the vectors $|\lambda_3\mu_3;\ \alpha_3\rangle_c$ are orthonormal. The representation $\mathfrak{D}^{\lambda_3\mu_3}$ associated with $\chi^{(k)}_{\alpha_3}$ is unitary and irreducible, hence, according to Schur's lemma, [Eq. (2.15)]

$$(\chi^{(k)}_{\alpha_3},\ \chi^{(k')}_{\alpha_3'})$$

[31] The method of labeling orthogonal spaces $\mathfrak{Q}^{(k)}_{\lambda_1\mu_1\lambda_2\mu_2}$ is discussed in Sec. 3C.

is independent of the row label α_3. Thus,

$$(h_k, h_{k'}) = d(k, k'; \lambda_3\mu_3) \sum_{\alpha_3} \cdot 1 = N_3\, d(k, k'; \lambda_3\mu_3) = \delta_{kk'}, \tag{3.12}$$

since, by assumption, the invariants h_k are orthonormal. Thus, if h_k, $k = 0, 1, \cdots, g-1$, is orthonormal with respect to the index k, then by Eq. (3.12), so is $\chi^{(k)}_{\alpha_3}$. The base vectors $|\lambda_3\mu_3;\, \alpha_3\rangle_k$ have unit norm, so that

$$|\lambda_3\mu_3;\, \alpha_3\rangle_k = (N_3)^{\frac{1}{2}}\chi^{(k)}_{\alpha_3} \tag{3.13}$$

are the orthonormal functions in

$$\mathfrak{Q}^{(k)}_{\lambda_1\mu_1\lambda_2\mu_2}$$

associated with the irreducible representation

$$\mathfrak{D}^{\lambda_3\mu_3}(U).$$

The $3(\lambda\mu)$ coefficients may be defined

$$h_k \equiv \sum_{\alpha_i} \begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{Bmatrix}_k \times |\lambda_1\mu_1;\, \alpha_1\rangle\, |\lambda_2\mu_2;\, \alpha_2\rangle\, |\lambda_3\mu_3;\, \alpha_3\rangle_c. \tag{3.14}$$

The $3(\lambda\mu)$ coefficients provide that linear combination of triple-product functions $|\lambda_1\mu_1;\, \alpha_1\rangle \mid \lambda_2\mu_2;\, \alpha_2\rangle\, |\lambda_3\mu_3;\, \alpha_3\rangle_c$ which yield an invariant h_k in the triple-product space. From Eqs. (3.9) and (3.13),

$$|\lambda_3\mu_3;\, \alpha_3\rangle_k = (N_3)^{\frac{1}{2}} \times \sum_{\alpha_1\alpha_2} \begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{Bmatrix}_k |\lambda_1\mu_1;\, \alpha_1\rangle\, |\lambda_2\mu_2;\, \alpha_2\rangle. \tag{3.15}$$

The $3(\lambda\mu)$ coefficients, defined by Eq. (3.14), when multiplied by $(N_3)^{\frac{1}{2}}$, yield the standard coupling coefficients. If the invariants h_k are given, the explicit evaluation of the $3(\lambda\mu)$ symbol involves taking the inner product of h_k with the triple-product vector

$$\begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{Bmatrix}_k = (|\lambda_1\mu_1;\, \alpha_1\rangle\, |\lambda_2\mu_2;\, \alpha_2\rangle\, |\lambda_3\mu_3;\, \alpha_3\rangle_c,\, h_k). \tag{3.16}$$

Thus, the evaluation of the $3(\lambda\mu)$ coefficients is reduced to the construction of an invariant h_k in the triple-product space, and as we see in the next two sections, this is not a difficult task.

B. $3(\lambda\mu)$ symbol for the nondegenerate case[32]: $\mathfrak{D}^{\lambda_1\mu_1} \otimes \mathfrak{D}^{\lambda_2\mu_2}$

Notation: Associate the variables (ζ_1, ζ_2), (ζ_3, ζ_4), (ζ_5, ζ_6), with the base vectors $|\lambda_1\mu_1;\, \alpha_1\rangle$, $|\lambda_2\mu_2;\, \alpha_2\rangle$, $|\lambda_3\mu_3;\, \alpha_3\rangle_c$, respectively. Label the 2×2 antisymmetric forms:

$$\delta_{ij} = (\delta^{(1)}_{ij}\ \delta^{(2)}_{ij},\ \delta^{(3)}_{ij}) = (\eta_i\sigma_j - \eta_j\sigma_i,\ \sigma_i\xi_j - \sigma_j\xi_i,\ \xi_i\eta_j - \xi_j\eta_i). \tag{3.17}$$

The most general invariant h_k may be constructed from a linear combination of products of 3×3 determinants. The following conditions must be imposed on h_k:

$$\text{(i)}\ T_{12}h_k = 0, \quad T_{34}h_k = 0, \quad T_{56}h_k = 0, \tag{3.18}$$

since h_k is of the form Eq. (3.14). By inspection of Eq. (2.10a), one sees that $|\lambda_1 0;\, \alpha_1\rangle$ is independent of δ_{12}. Hence h_k must not contain δ_{12}, and $T_{12}h_k = 0$ is satisfied automatically. h_k may then have the form

$$h_k = \sum_{k_i} \beta_k(k_i)[\zeta_1\cdot(\zeta_3 \times \zeta_5)]^{k_0} \times (\zeta_3\cdot\delta_{56})^{k_3}(\zeta_1\cdot\delta_{34})^{k_2}(\zeta_5\cdot\delta_{34})^{k_5}. \tag{3.19}$$

(ii) From the requirement that h_k be in the space

$$\mathfrak{Q}_{\lambda_1 0\lambda_2\mu_2\mu_3\lambda_3},$$

the degree conditions follow

$$k_1 + k_2 = \lambda_3,\ k_0 + k_2 + k_5 = \lambda_1,\ k_i \geq 0,\ k_0 + k_6 = \mu_3,\ k_0 + k_1 = \lambda_2,\ k_5 + k_6 = \mu_2. \tag{3.20}$$

This may be rewritten in the form

$$k_2 = P - (\lambda_2 + \mu_2),\ k_0 = P - (\lambda_3 + \mu_2),\ k_5 = P - (\lambda_3 + \mu_3),\ k_1 + k_2 = \lambda_3,\ k_5 + k_6 = \mu_2, \tag{3.21a}$$

where

$$P = k_0 + k_1 + k_2 + k_5 + k_6 = \tfrac{1}{3}(\lambda_1 + \lambda_2 + 2\mu_2 + 2\lambda_3 + \mu_3). \tag{3.21b}$$

From Eq. (3.21), the partition numbers λ_1, $[\lambda_2\mu_2]$, $[\lambda_3\mu_3]$, uniquely specify the integers k_i, $g(\lambda_i\mu_i) = 1$. Redefine the coefficient $\beta_k(k_i)$. Eq. (3.19) becomes

$$h(k_i) = \Delta(k_i)\, \frac{[\zeta_1\cdot(\zeta_3 \times \zeta_5)]^{k_0}(\zeta_3\cdot\delta_{56})^{k_1}(\zeta_1\cdot\delta_{56})^{k_2}(\zeta_1\cdot\delta_{34})^{k_5}(\zeta_5\cdot\delta_{34})^{k_6}}{k_0!\qquad k_1!\qquad k_2!\qquad k_5!\qquad k_6!}, \tag{3.22}$$

[32] The general expression for $[\lambda,\mu] \otimes [k,0]$ has been derived by M. Moshinsky, Rev. Mod. Phys. **34**, 813 (1962) in terms of a finite series.

$\Delta(k_i)$ normalizes the inner product $[h(k_i), h(k_i)]$ to unity, and is evaluated in Appendix B. The result is

$$[h(k_i), h(k_i')] = [\Delta(k_i)]^2 \delta_{k_i k'_i} \frac{(P+2)!\,(k_0+k_1+k_2+1)!\,(k_0+k_1+k_6+1)(k_0+k_5+k_6+1)!}{2k_0!\,k_1!\,k_2!\,k_5!\,k_6!\,(k_0+k_1+1)!\,(k_0+k_6+1)!}. \quad (3.23)$$

Since $h(k_i)$ is orthogonal, there exists N_3 orthonormal base vectors

$$|\lambda_3\mu_3;\alpha_3\rangle \quad \text{in} \quad \mathfrak{D}_{\lambda_1 0\lambda_2\mu_2},$$

corresponding to each set of values k_i, provided that k_i satisfy conditions (3.21). To determine whether the decomposition is complete, sum over the number of reduced direct-product vectors consistent with the constraints on k_i:

$$\begin{aligned} n &= \sum_{\lambda_1} N_3 = \tfrac{1}{2}\sum (\lambda_3+1)(\mu_3+1)(\lambda_3+\mu_3+2) \\ &= \tfrac{1}{2}\sum_{k_3=0}^{\lambda_1}\sum_{k_5=0}^{\lambda_1-k_3} (\lambda_2+1+k_2-k_3) \\ &\qquad \times (\mu_2-\lambda_1+1+k_2+2k_3) \\ &\qquad \times (\lambda_2+\mu_2+2+2k_2+k_3) \\ &= \tfrac{1}{2}(\lambda_1+1)(\lambda_1+2)\tfrac{1}{2}(\lambda_2+1)(\mu_2+1)(\lambda_2+\mu_2+2) \\ &= N_1N_2. \end{aligned}$$

The number of base vectors $|\lambda_3\mu_3;\alpha_3\rangle$ in $\mathfrak{D}_{\lambda_1 0\lambda_2\mu_2}$ is N_1N_2, and since this is the dimension of the space, the reduction is complete.

The inner product of $h(k_i)$, Eq. (3.22), and the triple-product vector yields the $3(\lambda\mu)$ symbol for the nondegenerate case. $h(k_i)$ must be expanded, constraints from the integration [see Eq. (1.2)] must be applied, and (using binomial identities) the sums must be contracted. The details are quite tedious and only the results are given here.[33]

$$\begin{Bmatrix} \lambda_1 0 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_1 & \alpha_2 & \alpha_3' \end{Bmatrix} = C \sum_{a\cdots e} \frac{(-1)^{a+b+e}(\lambda_3+1+k_0+b-c)!}{a!\,(k_5-a)!\,(\mu_3-q_3-b)!\,c!\,d!\,(p_3-d)!\,(\lambda_3-p_3-k_2+d)!}$$

$$\times \frac{(\lambda_3+\mu_3+1-k_2+d)!}{[-(\mu_3-q_3)+\lambda_1-p_1-a+b]!\,(\mu_3+p_3+1-k_6+\mu_2-q_2-c-d)!\,[-(\mu_3-q_3)+k_6-k_2+\lambda_1-p_1-a+c+d]!}$$

$$\times \frac{[\mu_3-q_3+k_2+k_5-(\lambda_1-p_1)-b-d]!}{(\mu_2-q_2-e)!\,[\lambda_3+\mu_3-q_3+1+k_0-(\lambda_1-p_1)+a-c]!\,[\mu_3-q_3+k_2-(\lambda_1-p_1)+a-b-d]!\,(b-c-e)!}$$

$$\times \frac{(\mu_3+p_3-q_3-b-d)!}{e!\,[r-(\mu_2-q_2)+e]!\,(k_0+p_3-p_2-b-d+e)!\,(\mu_2+p_2-q_2-r-e)!}, \quad (3.24)$$

where

$$r = r_1 + r_2 = k_0 + \mu_2 - q_2 - (\mu_3 - q_3) \quad \text{from} \quad t_3 = (t_0)_1 + (t_0)_2, \quad \alpha_3' : t_3 = (t_0)_3,$$

$$p_1 + p_2 = 2k_0 + \mu_2 - q_2 + p_3 - (\mu_3 - q_3) \quad \text{from} \quad y_1 + y_2 = y_3,$$

and

$$C = \frac{(-1)^{k_0+r_1}\,\Delta(k_1)}{N(\lambda_1 0;\alpha_1)N(\lambda_2\mu_2;\alpha_2)N(\lambda_3\mu_3;\,y_3t_3t_3)}\,\frac{r!}{r_1!\,r_2!}$$

$$\times \frac{(\mu_3+p_3-q_3+1)!\,(\mu_2+p_2-q_2+1)!\,(\mu_2+p_2-q_2-r_2)!}{(\mu_3+p_3+1)!\,(\lambda_3+\mu_3-q_3+1)!\,(\mu_2+p_2-q_2)!}. \quad (3.25)$$

$N(\lambda_i\mu_i;\,\alpha_i)$ is given by Eq. (2.10b) and $\Delta(k_i)$ by Eq. (3.23). For $\mu_2 = 0$, Eq. (3.24) reduces to one sum and for the two special cases where α_3 is minimum or maximum,

(i) $\alpha_{3_m} = [y_{3\min}, t_{3\min}, (t_0)_3 = -t_{3\min}]$,

$$p_3,\ q_3 = 0, \qquad r_3 = 2t_3,$$

(ii) $\alpha_{3M} = [y_{3\max}, t_{3\max}, (t_0)_3 = t_{3\max}]$,

$$p_3 = \lambda_3, \qquad q_3 = \mu_3, \qquad r_3 = 0,$$

the above expression reduces to a single factor. Let the phase convention for the $3(\lambda\mu)$ symbol be the

[33] Aside from the general expression for $[\lambda,\mu] \otimes [k,0]$ derived by Moshinsky (Ref. 32), other special cases appear in the literature, e.g., Hecht (Ref. 14) has coefficients for the special cases $[\lambda,\mu] \otimes$ [2,0], [0,2], [4,0], [2,1], [1,1] in terms of single factors. N. Mukunda and L. K. Pandit, J. Math. Phys. **6**, 1547 (1965) have closed expressions for the product $[\lambda,\mu] \otimes$ [3,0]. Coefficients of use to high-energy physicists have been constructed by S. Sawada and M. Yonezawa, Progr. Theoret. Phys. (Kyoto) **23**, 662 (1960); A. R. Edmonds, Proc. Roy. Soc. (London) **A268**, 567 (1962); M. A. Rashid, Nuovo Cimento **26**, 118 (1962); and J. J. de Swart (Ref. 20), among others.

following[34]:

$$\begin{Bmatrix} \lambda_1 0 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_{1M} & \alpha_2' & \alpha_{3M} \end{Bmatrix} > 0. \tag{3.26}$$

Case (ii) then allows us to determine the correct phase factor:

$$\begin{Bmatrix} \lambda_1 0 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_1 & \alpha_2 & \alpha_{3M} \end{Bmatrix} = \frac{(-1)^{\lambda_1 - p_1 + r_1 + k_0}\,\Delta(k_i)}{N(\lambda_1 0;\alpha_1)N(\lambda_2\mu_2;\alpha_2)N(\lambda_3\mu_3;\alpha_{3M})}$$

$$\times \frac{(\mu_2 + p_2 - q_2 + 1)!\,(\mu_2 + p_2 - q_2 - r_2)!\,r!}{(\mu_2 - q_2)!\,(\mu_2 + p_2 - q_2)!\,k_0!\,k_2!\,k_6!\,(\lambda_1 - p_1)!\,(\lambda_2 - p_2)!\,(\lambda_2 + \mu_2 - q_2 + 1)!\,[k_1 - (\lambda_2 - p_2)]!\,r_1!\,r_2!}. \tag{3.27}$$

If $\alpha_1 = \alpha_{1M}$, it is clear the $3(\lambda\mu)$ symbol must be multiplied by $(-1)^{k_0}$ to satisfy the convention, Eq. (3.26).

C. $3(\lambda\mu)$ symbol for the degenerate case: $\mathfrak{D}^{\lambda_1\mu_1} \otimes \mathfrak{D}^{\lambda_2\mu_2}$

To determine the $3(\lambda\mu)$ coefficients uniquely, it is necessary to determine the invariants $h_k(k_i)$ uniquely. In Sec. (1) below, conditions are placed on the invariant, but, unlike the previous case, the invariant is still not uniquely determined. Linear combinations of the invariants are possible, and in Sec. 2, two methods are employed to orthogonalize and uniquely determine the invariants. The explicit expression and completeness of reduction then follow, as in Sec. 3B above.

1. Form of invariant

The following conditions must be imposed on the invariant $h_k(k_i)$:

$$(\alpha) \quad T_{12}h_k = 0, \qquad T_{34}h_k = 0, \qquad T_{56}h_k = 0,$$

since the invariant has the form Eq. (3.13). The most general invariant h_k must then have a summand of the form

$$\beta_k(k_i)[\zeta_1\cdot(\zeta_3 \times \zeta_5)]^{k_0}F(k_i)[\delta_{12}\cdot(\delta_{34} \times \delta_{56})]^{k_0'}, \tag{3.28a}$$

where

$$F(k_i) = (\zeta_3\cdot\delta_{56})^{k_1}(\zeta_1\cdot\delta_{56})^{k_2}(\zeta_5\cdot\delta_{12})^{k_3} \times (\zeta_3\cdot\delta_{12})^{k_4}(\zeta_1\cdot\delta_{34})^{k_5}(\zeta_5\cdot\delta_{34})^{k_6}. \tag{3.28b}$$

(β) Since h_k is a member of the space

$$\mathfrak{Q}^{(k)}_{\lambda_1\mu_1\lambda_2\mu_2\mu_3\lambda_3},$$

$$k_0 + k_3 + k_6 = \mu_3, \quad k_0' + k_1 + k_2 = \lambda_3,$$
$$k_0 + k_1 + k_4 = \lambda_2, \quad k_0 + k_5 + k_6 = \mu_2, \quad k_i \geq 0,$$
$$k_0 + k_2 + k_5 = \lambda_1, \quad k_0 + k_3 + k_4 = \mu_1. \tag{3.29}$$

From Eq. (3.29), it may be noted that

$$k_0 - k_0' = P - (\mu_1 + \mu_2 + \lambda_3), \tag{3.30a}$$

where

$$P = k_0 + k_1 + \cdots + k_6 + 2k_0' = \tfrac{1}{3}(\lambda_1 + 2\mu_1 + \lambda_2 + 2\mu_2 + 2\lambda_3 + \mu_3). \tag{3.30b}$$

The requirement that the invariant h_k lies in the triple-product space

$$\mathfrak{Q}^{(k)}_{\lambda_1\mu_1\lambda_2\mu_2\mu_3\lambda_3},$$

[Eqs. (3.29) and (3.30)] allows for a range of values of k_i instead of a unique set, as in the previous case, and this gives rise to the multiplicity problem.

The terms of the summation, Eq. (3.28), are not independent because of the identity

$$[\zeta_1\cdot(\zeta_3 \times \zeta_5)][\delta_{12}\cdot(\delta_{34} \times \delta_{56})] = H_1 + H_2, \tag{3.31a}$$

where

$$H_1 = (\zeta_3\cdot\delta_{56})(\zeta_5\cdot\delta_{12})(\zeta_1\cdot\delta_{34}), \qquad H_2 = (\zeta_1\cdot\delta_{56})(\zeta_3\cdot\delta_{12})(\zeta_5\cdot\delta_{34}). \tag{3.31b}$$

To require that the invariant h_k be a sum over linearly independent terms, set

$$\text{(i)}\ k_0' = 0, \quad \text{for} \quad k_0 - k_0' = P - (\mu_1 + \mu_2 + \lambda_3) \geq 0, \qquad \text{(ii)}\ k_0 = 0, \quad \text{for} \quad k_0 - k_0' < 0. \tag{3.32}$$

If the largest common term, $F(\rho_i)$, is then factored from the sum, the invariant $h_k(\rho_i)$ may be put in the form

$$h_k(\rho_i) = [\zeta_1\cdot(\zeta_3 \times \zeta_5)]^{k_0}F(\rho_i)\sum \beta_k(\rho_i;n_1,n_2)(H_1)^{n_1}H_2^{n_2}, \quad n_1 + n_2 = N \tag{3.33}$$

[34] This phase convention, the choice of α_{1M}, α_{3M}, agrees with most authors, but the definition of highest weight state differs, e.g., since Hecht (Ref. 14), Elliott (Ref. 12), and Elliott (Ref. 13) have $-Y$, they would be considering the minimum Y state, compared to the notation of this paper. de Swart (Ref. 20) and Kuriyan, *et al.* (Ref. 22) choose $I_z = I_{\max}$ (and associated Y) as the highest weight state.

for $k_0 - k_0' \geq 0$. For $k_0 - k_0' < 0$, the invariant h_k becomes

$$h_k(\rho_i) = [\delta_{12}\cdot(\delta_{34} \times \delta_{56})]^{k'_0} \times F(\rho_i) \sum \epsilon_k(\rho_i; n_1, n_2) H_1^{n_1}(H_2)^{n_2}, \quad n_1 + n_2 = N, \tag{3.34}$$

where $k = 0, 1, \cdots, N = g - 1$ and $k_i = \rho_i + n_1$, $i = 1, 3, 5$; $k_i = \rho_i + n_2$, $i = 2, 4, 6$ and with the conditions

$$\begin{aligned} &k_0 + \rho_3 + \rho_6 + N = \mu_3, \quad k_0' + \rho_1 + \rho_2 + N = \lambda_3, \\ &k_0 + \rho_1 + \rho_4 + N = \lambda_2, \quad k_0' + \rho_5 + \rho_6 + N = \mu_2, \\ &k_0 + \rho_2 + \rho_5 + N = \lambda_1, \quad k_0' + \rho_3 + \rho_4 + N = \mu_1. \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \rho_i \geq 0, \end{aligned} \tag{3.35}$$

According to Eq. (3.32), k_0 or k_0' equals zero in Eq. (3.35), depending on the sign of the difference.

The exact expression for $N + 1 = g$,[35] the number of times the irreducible representation $\mathfrak{D}^{\lambda_3\mu_3}$ is contained in the direct-product representation $\mathfrak{D}^{\lambda_1\mu_1} \otimes \mathfrak{D}^{\lambda_2\mu_2}$, is quite complicated if simple inequalities are assumed on the partition numbers $[\lambda_i\mu_i]$. Conversely, if complicated bounds are imposed on P, then the expression for N is simple. Write the conditions (3.35) in the alternate form

$$\begin{aligned} \rho_4 - \rho_6 &= P - (\mu_2 + \lambda_3 + \mu_3), \\ \rho_5 - \rho_3 &= P - (\mu_1 + \lambda_3 + \mu_3), \\ \rho_2 - \rho_4 &= P - (\mu_1 + \lambda_2 + \mu_2), \\ \rho_3 - \rho_1 &= P - (\lambda_2 + \mu_2 + \lambda_3), \\ \rho_6 - \rho_2 &= P - (\lambda_1 + \mu_1 + \lambda_3), \\ \rho_1 - \rho_5 &= P - (\lambda_1 + \mu_1 + \mu_2). \end{aligned} \tag{3.36}$$

Equations (3.36), (3.30), and one relation of Eq. (3.35) constitute the alternate set to Eqs. (3.35). $N = n_1 + n_2$ is chosen such that there is one unique set of values ρ_i. At least two ρ_i equal zero, one for $i = 1, 3, 5$, and one for $i = 2, 4, 6$, respectively, depending on the value of N. From Eq. (3.36) the expressions for g follow:

$$\begin{aligned} &\rho_2 = 0, \quad \rho_4 = \lambda_2 + \mu_2 + \mu_1 - P, \quad k_0 \geq 0, \\ &\qquad \rho_6 = P - (\lambda_1 + \mu_1 + \lambda_3), \quad \rho_i \geq 0 \end{aligned} \tag{3.37}$$

and Case I:

$$\begin{aligned} \rho_1 &= 0, \qquad N = \lambda_3, \\ \rho_3 &= P - (\lambda_2 + \mu_2 + \lambda_3), \\ \rho_5 &= \lambda_1 + \mu_1 + \mu_2 - P, \end{aligned}$$

Case II:

$$\begin{aligned} \rho_3 &= 0, \qquad N = P - (\lambda_2 + \mu_2), \\ \rho_1 &= \lambda_2 + \mu_2 + \lambda_3 - P, \\ \rho_5 &= P - (\mu_1 + \lambda_3 + \mu_3), \end{aligned}$$

or Case III:

$$\begin{aligned} \rho_5 &= 0, \\ \rho_1 &= P - (\lambda_1 + \mu_1 + \mu_2), \\ N &= \mu_1 + \lambda_1 + \mu_2 + \lambda_3 - P, \\ \rho_3 &= \mu_1 + \lambda_3 + \mu_3 - P. \end{aligned}$$

The other possible bounds on P, and expressions for N, are obtained by exchanging $(\lambda_1\mu_1) \leftrightarrow (\lambda_2\mu_2)$ and $(\lambda_1\mu_1) \leftrightarrow (\mu_3\lambda_3)$ along with the corresponding changes of ρ_i [see Sec. 3D]. Altogether there are nine possibilities. When $k_0' > 0$, the correct degeneracy expression, N, is obtained from Eq. (3.37) by exchanging $\lambda_i \leftrightarrow \mu_i$ and making the corresponding changes in ρ_i [see Eq. (3.66)].

2. *Determination of* $\beta_k(\rho_i; n_1, n_2)$

Given the invariants Eqs. (3.33) and (3.34), the problem still remains to uniquely specify the g^2 coefficients $\beta_k(\rho_i; n_1, n_2)$. Orthogonality of the invariants $h_k(\rho_i)$ provides $\frac{1}{2}g(g-1)$ conditions, normalization g conditions, thus $\frac{1}{2}g(g+1)$ conditions in all on the g^2 coefficients. Any set of coefficients $\beta_k(\rho_i; n_1, n_2)$ may be related to another set $\beta_k'(\rho_i; n_1, n_2)$ through the transformation

$$\beta_k'(\rho_i; n_1, n_2) = \sum_{\sigma=0}^{N} B_{k\sigma}\beta_\sigma(\rho_i; n_1, n_2) \tag{3.38}$$

or

$$h_k'(\rho_i) = \sum_{\sigma=0}^{N} B_{k\sigma} h_\sigma(\rho_i), \qquad k = 0, 1, \cdots, N.$$

This implies, from Eq. (3.14), that

$$\begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{Bmatrix}_k' = \sum B_{k\sigma} \begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{Bmatrix}_\sigma. \tag{3.39}$$

[35] B. Preziosi, A. Simoni, and B. Vitale, Nuovo Cimento 34, 1101 (1964), have calculated g from a straightforward multiplication of Young tableaus. Other methods for determining the degeneracy g appear in the literature. Freudenthal's formula, an implicit formula in terms of a recursion relation, appears in N. Jacobson, *Lie Algebras* (Interscience Publishers, Inc., New York, 1962). The formula is derived by relating the weight and multiplicity structure of $SU(3)$ [also $SU(n)$]. J. P. Antoine and D. Speiser, J. Math. Phys. 5, 1226 (1964); 5, 1560 (1964), describe graphical methods for general simple compact Lie groups. S. Gasiorowicz, "A Simple Graphical Method in the Analysis of $SU(3)$," Argonne Report ANL-6729, is a review article of the Speiser method for $SU(3)$.

If the new set of invariants $h'_k(\rho_i)$ are orthonormalized, and if the $3(\lambda\mu)$ coefficients are chosen real, then B_{ij} is an orthogonal transformation.

Two methods are now discussed to uniquely specify the coefficients $\beta_k(\rho_i; n_1, n_2)$ and form orthogonal states $h_k(\rho_i)$.[36]

3. Moshinsky's operator X

Moshinsky has constructed an Hermitian operator[37] X

$$X = \sum T_{\alpha+2,\beta}T_{\beta\rho}T_{\rho,\alpha+2}, \quad \alpha, \beta, \rho = 1, 2, \tag{3.40}$$

which commutes with the operators

$$T_{12}, T_{34}, T_{56}, T_{ii}, \qquad i = 1, \cdots, 6,$$

and the generators M_{ij}, and which combines the variables of the separate spaces[38]

$$\mathfrak{Q}_{\lambda_1\mu_1}, \mathfrak{Q}_{\lambda_2\mu_2}.$$

The invariant $h_k(\rho_i)$ must then be diagonalized with respect to X

$$Xh_k(\rho_i) = x_k(\rho_i)h_k(\rho_i). \tag{3.41}$$

The eigenvalues $x_k(\rho_i)$ are, of course, real, and Moshinsky[37] has shown that they are distinct.

The operator X, operating on the summand of Eq. (3.33), yields

$$\begin{aligned} &X\{[\zeta_1\cdot(\zeta_3 \times \zeta_5)]^{k_0}F(\rho_i)(H_1)^{n_1}H_2^{n_2}\} \\ &= [\zeta_1\cdot(\zeta_3 \times \zeta_5)]^{k_0}F(\rho_i) \\ &\times [f(\rho_i; n_1, n_2)H_1^{n_1}H_2^{n_2} + g(\rho_i; n_1, n_2) \\ &\times (H_1)^{n_1-1}H_2^{n_2+1} + h(\rho_i; n_1, n_2)H_1^{n_1+1}H_2^{n_2-1}], \end{aligned} \tag{3.42}$$

where

$$\begin{aligned} &f(\rho_i; n_1, n_2) \\ &= (\mu_1 + 1)!\,[\mu_2(\mu_1 + 2) + (k_3 + 1)(k'_0 + k_1)] \\ &\quad + (\lambda_1 + \mu_1 + 3)[k_1(k_2 + 1) + k_6(k'_0 + k_2 + k_3 + 2)] \\ &\quad + k_1k_3(k_2 + 1) + k_4k_6(k_0 + k_2 + 1) \end{aligned} \tag{3.43a}$$

and

$$g(\rho_i; n_1, n_2) = -k_1k_3k_5, \qquad h(\rho_i; n_1, n_2) = k_2k_4k_6. \tag{3.43b}$$

Similarly, X on a summand of Eq. (3.34) has the same form as Eq. (3.42), but

$$\begin{aligned} &f'(\rho_i; n_1, n_2) = f(\rho_i; n_1, n_2)\,|_{k_0=0} \\ &+ k'_0[k'_0k_2 + (\mu_1 + 2)(\mu_2 + 2) + k_1(k_2 + 1) \\ &+ (\lambda_1 + \mu_1 + 1)(k_1 + k_2 + k_3 + k_4 + 2) + 3k_6 \\ &+ 2k_1 + k_1k_3 + k_2k_6 + k_3k_6 + k_1k_5 - 2k_2] \end{aligned} \tag{3.44}$$

and $g(\rho_i; n_1, n_2)$, $h(\rho_i; n_1, n_2)$ are given by Eq. (3.43b).

A secular determinant, obtained from Eq. (3.41), must be solved for the eigenvalues $x_k(\rho_i)$ to determine the coefficients $\beta_k(\rho_i; n_1, n_2)$. Given the coefficients $\beta_k(\rho_i; n_1, n_2)$, the $3(\lambda\mu)$ coefficients are found by taking the inner product of $h_k(\rho_i)$ with the triple product vector [see Eq. (3.16)]. The general $3(\lambda\mu)$ coefficient, in terms of the $\beta_k(\rho_i; n_1, n_2)$ is then Eq. (3.48).

The symmetry relations of the $3(\lambda\mu)$ coefficients are not obvious from the form of the operator X, Eq. (3.40). If the simple case $g = 2$ is considered, e.g.,

$$[1, 1] \times [1, 1] = 2[1, 1] + \cdots,$$

the standard convention is to choose the $3(\lambda\mu)$ coefficients such that under the various symmetry operations, one coefficient is symmetric, the other antisymmetric. The $3(\lambda\mu)$ coefficients determined by X do not have this property.

4. Choice of $\beta_k(\rho_i; n_1, n_2)$

To require that the $3(\lambda\mu)$ coefficients have simple symmetry properties, let the $\beta_k(\rho_i; n_1, n_2)$ be chosen such that

$$\beta_k(\rho_i; n_1, n_2) = (-1)^k\beta_k(\rho_i; n_2, n_1) \tag{3.45}$$

for $k = 0, 1, \cdots, N$. The condition (3.45) separates the invariants $h_k(\rho_i)$ into states which are even or odd under the various permutation operations on the variables. The odd, even, states are then mutually orthogonal. To finally determine the coefficients $\beta_k(\rho_i; n_1, n_2)$ a Gram–Schmidt orthogonalization procedure may be employed. Divide the coefficients $\beta_k(\rho_i; i, j)$ by the normalization $\beta_k(\rho_i; N, 0)$,

$$a_{kj} = \beta_k(\rho_i; i, j)/\beta_k(\rho_i; N, 0), \qquad k = 0, 1, \cdots, N \tag{3.46}$$

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[36] The row and state labeling problem has been discussed by G. E. Baird and L. C. Biedenharn in a series of papers: J. Math Phys. 4, 1449 (1963); 5, 1723 (1964); 5, 1730 (1964). In particular, they show the interesting result that the multiplicity structure of $SU(n)$ operators may be put into a one-to-one association with the multiplicity structure of the corresponding states.

[37] M. Moshinsky, J. Math. Phys. 4, 1128 (1963).

[38] L. O'Raifeartaigh and A. J. Macfarlane (to be published) have constructed an operator from the generators of $SU(3)$. Professor Moshinsky has pointed out in discussion that this operator differs from the operator X only by Casimir operators. Other operators satisfying the above conditions may, of course, also be constructed.

and choose the coefficients a_{ki} so that the invariants $h_k(\rho_i)$ have the form

$$h_k(\rho_i) = [\zeta_1\cdot(\zeta_3 \times \zeta_5)]^{k_0} \times F(\rho_i)\beta_k \sum_{\alpha=0}^{[k/2]} a_{k\alpha}(H_1H_2)^\alpha(H_1^{k-2\alpha} \pm (H_2)^{k-2\alpha}), \quad (3.47)$$

where $a_{k0} = 1$ and $\pm$ refer to k even, odd, respectively, e.g.,

$$h_0(\rho_i) = [\zeta_1\cdot(\zeta_3 \times \zeta_5)]^{k_0}F(\rho_i)\beta_0(H_1^N + H_2^N),$$

$$h_2(\rho_i) = [\zeta_1\cdot(\zeta_3 \times \zeta_5)]^{k_0}F(\rho_i)\beta_2 \times [(H_1^N + H_2^N) + a_{21}(H_1H_2)(H_1^{N-2} + H_2^{N-2})].$$

The factors β_k are normalizations and the coefficients a_{ki} are uniquely determined by integration, the necessary integrations being performed in Appendix B.

5. Explicit expression

The inner product of the invariant $h_k(\rho_i)$, Eq. (3.33), with the triple product vector [see Eq. (3.16)] yields the $3(\lambda\mu)$ coefficient in terms of the coefficients[39] $\beta_k(\rho_i; n_1, n_2)$:

$$\begin{Bmatrix}\lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_3\mu_3\\ \alpha_1 & \alpha_2 & \alpha_3'\end{Bmatrix}_k = (-1)^\phi \sum \beta_k(\rho_i; n_1, n_2) \frac{\prod_i k_i!\, k_0!\, (-1)^{m_{03}+m_{04}+m_{05}}}{\prod_{ij} n_{ij}! \prod_s m_{0s}!} \times \prod_{i=1,2} S(\lambda_i\mu_i; \alpha_i)S(\mu_3\lambda_3; -\alpha_3'),^{40} \quad (3.48)$$

$$\phi = \mu_3 + k_0 + q_1 + q_2, \qquad \alpha_3' : r_3 = 0,$$

where

$$S(\lambda_i\mu_i; \alpha_i) = M(\lambda_i\mu_i; \alpha_i) \sum_{u_i} \frac{(-1)^{u_i+n_i+m_i} m_i!\, n_i!\, (p_i - r_i + m_i)!}{(p_i + m_i + n_i + 1)!\, u_i!\, (p_i - n_i)!\, (p_i - r_i + m_i - n_i)!} \times \frac{[r_i - (\mu_i - q_i) + n_i]!}{(-p_i + r_i + u_i)!\, (\mu_i + p_i - q_i - r_i - u_i)!\, [n_i - (\mu_i - q_i) - p_i + r_i + u_i]!} \quad (3.49a)$$

and

$$M(\lambda_i\mu_i; \alpha_i) = \frac{(\mu_i + p_i - q_i + 1)!\, (\mu_i + p_i - q_i - r_i)!}{(\mu_i + p_i - q_i)!\, N(\lambda_i\mu_i; \alpha_i)}. \quad (3.49b)$$

The following constraints must be applied to Eq. (3.48):

$$n_1 = n_{31} + n_{41}, \quad n_2 = n_{51} + n_{61}, \quad i = 1, 3, 5,$$
$$n_3 = n_{11} + n_{21}, \quad k_i = \rho_i + n_1,$$
$$m_1 = n_{32} + n_{42}, \quad m_2 = n_{52} + n_{62}, \quad i = 2, 4, 6,$$
$$m_3 = n_{12} + n_{22}, \quad k_i = \rho_i + n_2,$$
$$\sum_{j=1}^{3} n_{ij} = k_i, \quad i = 1, \cdots, 6, \qquad \sum_{s=1}^{6} m_{0s} = k_0,$$
$$r = r_1 + r_2 = k_0 + \mu_2 - q_2 + \mu_1 - q_1 - (\mu_3 - q_3),$$
$$p_1 + p_2 = 2k_0 - \mu_3 + p_3 + q_3 + \mu_1 - q_1 + \mu_2 - q_2,$$
$$p_3 + q_3 = m_{01} + m_{04} + n_{33} + n_{63} + m_3 + n_3,$$
$$\lambda_1 + \mu_1 - (p_1 + q_1) = m_{05} + m_{06} + n_{23} + n_{53} + m_1 + n_1,$$
$$\mu_3 - q_3 = m_{02} + m_{05} + m_{32} + m_{62} - n_3,$$
$$-\mu_1 + q_1 + r_1 = m_{03} + m_{04} + n_{22} + n_{52} - n_1,$$
$$-p_3 = m_{03} + m_{06} + n_{31} + n_{61} - m_3,$$
$$p_1 - r_1 = m_{01} + m_{02} + n_{21} + n_{51} - m_1,$$
$$n_{13} + n_{43} + m_{02} + m_{03} + m_2 + n_2 = \lambda_2 + \mu_2 - (p_2 + q_2),$$
$$m_{04} + m_{05} + n_{11} + n_{41} - m_2 = p_2 - r_2,$$
$$m_{01} + m_{06} + n_{12} + n_{42} - n_2 = -\mu_2 + q_2 + r_2, \quad (3.49c)$$

$N(\lambda_i\mu_i; \alpha_i)$ is given by Eq. (2.10b).

The phase convention is that of Eq. (3.26). The necessary coefficient for this case is

$$\begin{Bmatrix}\lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_3\mu_3\\ \alpha_{1M} & \alpha_2' & \alpha_{3M}\end{Bmatrix}_k = C' \times \sum_{n_1+n_3=N} \frac{\beta_k(\rho_i; n_1, n_2)k_1!\, k_5!}{(\mu_2 + p_2 + 1 - k_6)!\, [-(\mu_2 - q_2) + k_5]!}, \quad (3.50a)$$

[39] Closed expressions for the coefficients for the direct product $[\lambda\mu] \otimes [1,1]$ have been given by Kuriyan *et al.* (Ref. 22) and Hecht (Ref. 14). T. A. Brody, M. Moshinsky, and I. Renero, J. Math. Phys. 6, 1540 (1965), have recursion relations to determine coefficients for general direct product $[\lambda_1\mu_1] \otimes [\lambda_2\mu_2]$.

[40] The choice α'_3, $r_3 = 0$, is made because the $3(\lambda\mu)$ coefficient, Eq. (3.48), may then be divided by the factor $((t_1), (t_0)_1; t_2(t_0)_2|t_1t_2t_3(t_0)_3 = t_3)$, the CG coefficient for $SU(2)$, and multiplied by $(N_3)^{1/2}$, to obtain the isoscalar factor, as defined by Edmonds (Ref. 33).

where

$$C' = \frac{(-1)^{k_0}(\mu_2 + p_2 - q_2 + 1)!}{N(\lambda_1\mu_1; \alpha_{1M})N(\lambda_2\mu_2; \alpha_2)N(\mu_3\lambda_3; \alpha_{3M})(\mu_2 - q_2)!\,(\mu_2 + p_2 - q_2)!} \tag{3.50b}$$

α_2' is $y_2 = \lambda_3 + 2\mu_3 - (\lambda_1 + 2\mu_1)$, $(t_0)_2 = \frac{1}{2}(\lambda_3 - \lambda_1)$, with t_2 assuming, according to Biedenharn's results,[36] g values for given α_{1M}, α_{3M}. To define a proper phase convention, a nonvanishing $3(\lambda\mu)$ coefficient must be made positive. However, the phase of $\beta_k(\rho_i; n_1, n_2)$ is, in general, undetermined. For $k = 0$, when $n_1 = N$, $n_2 = 0$, and $n_2 = N$, $n_1 = 0$, it is clear from Eq. (3.50) that the $3(\lambda\mu)$ coefficient must be multiplied by $(-1)^{k_0}$ to satisfy Eq. (3.26). In general, the $3(\lambda\mu)$ coefficient must be multiplied by $(-1)^{\phi}$, where ϕ is a function of the parameters k_i.

6. *Completeness of the reduction*

Equations (3.29) plus the restriction, Eq. (3.32), give g independent terms, appropriate linear combinations of which yield g orthonormal invariants $h_k(\rho_i)$, and, from Eq. (3.13), g orthonormal direct-product base vectors associated with the irreducible representations $\mathfrak{D}^{\lambda_3\mu_3}$. To determine completeness, sum over the reduced direct-product states:

$$\begin{aligned} n &= \sum gN_3 \\ &= \tfrac{1}{2}\sum g(\lambda_3 + 1)(\mu_3 + 1)(\lambda_3 + \mu_3 + 2) \end{aligned} \tag{3.51}$$

$n = n_a + n_b$, where n_a is the case $k_0 \geq 0$, and n_b is the case $k_0 < 0$, or

$$n = n_a + n_b' - n_0, \tag{3.52}$$

where n_b' are the terms $k_0 \leq 0$ and n_0 are the terms $k_0 = 0$. Instead of Eq. (3.51), the numbers k_i, Eq. (3.29), may be substituted for $\lambda_3\mu_3$; the sum over all possible k_i, using Eq. (3.32), then includes the degeneracy g. Note that

$$n_b' = n_a\,|_{\lambda_1\leftrightarrow\mu_1,\ \lambda_3\leftrightarrow\mu_3}.$$

The result of the summation is

$$\begin{aligned} n_a &= \tfrac{1}{8}(\lambda_1 + 1)(\mu_1 + 1)(\lambda_1 + 2)(\lambda_2 + \mu_2 + 2) \\ &\quad \times [\mu_1(\lambda_2 - \mu_2 + 1) + 2(\lambda_2 + 1)(\mu_2 + 1)], \\ n_0 &= \tfrac{1}{4}(\mu_1 + 1)(\lambda_1 + 1)(\lambda_2 + \mu_2 + 2) \\ &\quad \times [\lambda_1 + \lambda_1\mu_1 + \mu_1 + (\lambda_1 - \mu_1)(\mu_2 - \lambda_2) \\ &\qquad + 2(\lambda_2 + 1)(\mu_2 + 1)]. \end{aligned} \tag{3.53}$$

Putting Eqs. (3.53) into Eq. (3.52), one can then see that

$$n = \sum gN_3 = N_1 \cdot N_2.$$

Thus, the reduction of the direct-product representation is complete; the gN_3 product base vectors $|\lambda_3\mu_3;\ \alpha_3\rangle_k$, $k = 0, 1, \cdots, g - 1$, associated with the irreducible representation $\mathfrak{D}^{\lambda_3\mu_3}$, span the sum of the spaces $\mathfrak{Q}^{(k)}_{\lambda_1\mu_1\lambda_2\mu_2}$.

D. Symmetry of the $3(\lambda\mu)$ coefficients[41]

Let the operator P_{12} exchange the coordinates $(\zeta_1, \zeta_2) \leftrightarrow (\zeta_3, \zeta_4)$. Then, from Eq. (3.33) ($k_0 \geq 0$),

$$\begin{aligned} P_{12}h_k(\rho_i) &= (-1)^{k_0}[\zeta_1 \cdot (\zeta_3 \times \zeta_5)]^{k_0}[P_{12}F(\rho_i)] \\ &\quad \times \sum \beta_k(\rho_i; n_2, n_1)(H_1)^{n_1}H_2^{n_2}, \end{aligned}$$

using the fact that $P_{12}H_1 = H_2$. Let $\mathcal{P}_{12}$ be the operator which exchanges the parameters $\rho_1 \leftrightarrow \rho_2$, $\rho_3 \leftrightarrow \rho_6$, $\rho_4 \leftrightarrow \rho_5$. Using Eq. (3.28b), it may be seen that $\mathcal{P}_{12}P_{12}F(\rho_i) = F(\rho_i)$, and hence,

$$\begin{aligned} \mathcal{P}_{12}P_{12}h_k(\rho_i) &= (-1)^{k_0+k}[\zeta_1 \cdot (\zeta_3 \times \zeta_5)]^{k_0}F(\rho_i) \\ &\quad \times \sum \beta_k(\rho_i'; n_1, n_2)(H_1)^{n_1}H_2^{n_2}. \end{aligned}$$

If it can be shown that

$$\beta_k(\rho_i'; n_1, n_2) = \beta_k(\rho_i; n_1, n_2), \tag{3.54}$$

then the result follows

$$\mathcal{P}_{12}P_{12}h_k(\rho_i) = (-1)^{k_0+k}h_k(\rho_i). \tag{3.55}$$

Using Eq. (3.14),

$$\begin{aligned} &\mathcal{P}_{12}P_{12}h_k(\rho_i) \\ &= \sum \begin{Bmatrix} \lambda_2\mu_2 & \lambda_1\mu_1 & \lambda_3\mu_3 \\ \alpha_2 & \alpha_1 & \alpha_3 \end{Bmatrix}_k |\lambda_1\mu_1; \alpha_1\rangle\, |\lambda_2\mu_2; \alpha_2\rangle\, |\lambda_3\mu_3; \alpha_3\rangle_c. \end{aligned}$$

The relation

$$\begin{Bmatrix} \lambda_2\mu_2 & \lambda_1\mu_1 & \lambda_3\mu_3 \\ \alpha_2 & \alpha_1 & \alpha_3 \end{Bmatrix}_k = (-1)^{k_0+k}\begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{Bmatrix}_k \tag{3.56}$$

then holds. A similar result follows for $k_0' > 0$.

Likewise, let P_{13} be the exchange $(\zeta_1, \zeta_2) \leftrightarrow (\zeta_5, \zeta_6)$. It may be shown that

$$\mathcal{P}_{13}P_{13}h_k(\rho_i) = (-1)^{k_0+k}h_k(\rho_i) \tag{3.57}$$

[41] de Swart (Ref. 20) and Hecht (Ref. 14) have discussed symmetries for the case $g = 2$. J. R. Derome and W. T. Sharp, J. Math. Phys. **6**, 1584 (1965), have discussed symmetries for 3-j and 6-j symbols of a general group without specifying the phase or method of labeling degenerate states.

assuming Eq. (3.54), where $\mathcal{P}_{13}$ is the interchange of the labels

$$\rho_1 \leftrightarrow \rho_4, \qquad \rho_2 \leftrightarrow \rho_3, \qquad \rho_5 \leftrightarrow \rho_6. \tag{3.58}$$

From Eq. (3.57),

$$\begin{Bmatrix} \mu_3\lambda_3 & \lambda_2\mu_2 & \mu_1\lambda_1 \\ -\alpha_3 & \alpha_2 & -\alpha_1 \end{Bmatrix}_k = (-1)^{k_0+k} \begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{Bmatrix}_k. \tag{3.59}$$

Similarly, exchange of $(\zeta_3, \zeta_4) \leftrightarrow (\zeta_5, \zeta_6)$, P_{23}, and the interchange $\mathcal{P}_{23}$

$$\rho_1 \leftrightarrow \rho_6, \qquad \rho_2 \leftrightarrow \rho_5, \qquad \rho_3 \leftrightarrow \rho_4 \tag{3.60}$$

implies

$$\begin{Bmatrix} \lambda_1\mu_1 & \mu_3\lambda_3 & \mu_2\lambda_2 \\ \alpha_1 & -\alpha_3 & -\alpha_2 \end{Bmatrix}_k = (-1)^{k_0+k} \begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{Bmatrix}_k. \tag{3.61}$$

It is clear that Eq. (3.54) holds. The inner product $(h_0(\rho_i), h_2(\rho_i)) = 0$ determines $a_{21}(\rho_i, k_0)$.

$$a_{21}(\rho_i, k_0) = -\frac{[||^{k_0}F(\rho_i)(H_1^N + H_2^N), ||^{k_0}F(\rho_i)(H_1^N + H_2^N)]}{[||^{k_0}F(\rho_i)(H_1^N + H_2^N), ||^{k_0}F(\rho_i)(H_1H_2)(H_1^{N-2} + H_2^{N-2})]}. \tag{3.62}$$

Exchange the coordinates, then, Eq. (3.62) remains the same except $F(\rho_i)$ goes to $F'(\rho_i) = PF(\rho_i)$, where P stands for P_{12}, P_{13}, P_{23}. Next, exchange the parameters ρ_i, since

$$\mathcal{P}PF(\rho_i) = F(\rho_i), \qquad a_{21}(\rho_i, k_0) = a_{21}(\rho_i', k_0),$$

Eq. (3.54) then holds by induction. Assume that the coefficients $a_{ki}(\rho_i, k_0)$ (for k, N even), for $j < \frac{1}{2}k = (\frac{1}{2}N - 1), \cdots, 1, 0$, have the property that $a_{ki}(\rho_i, k_0) = a_{ki}(\rho_i', k_0)$. The inner product $(h_N(\rho_i), h_k(\rho_i)) = 0$, for $k = 0, 2, \cdots, N - 2$ provides $\frac{1}{2}N$ inhomogeneous equations for $a_{Ni}(\rho_i, k_0)$:

$$b_{kN}(\rho_i; k_0) + \sum_{\alpha=1}^{N/2} b_{k\alpha}a_{N\alpha}(\rho_i; k_0) = 0,$$

$$k = 0, 2, \cdots, N - 2.$$

Since, by assumption, $b_{ik}(\rho_i; k_0) = b_{ik}(\rho_i'; k_0)$,

$$a_{N\alpha}(\rho_i; k_0) = a_{N\alpha}(\rho_i'; k_0).$$

A similar argument applies to k odd.

The conjugation result follows similarly. Note first that

$$\mathcal{R}R\ |\lambda_1\mu_1; \alpha_1\rangle\ |\lambda_2\mu_2; \alpha_2\rangle\ |\lambda_3\mu_3; \alpha_3\rangle_c = A\ |\lambda_1\mu_1; \alpha_1\rangle\ |\lambda_2\mu_2; \alpha_2\rangle\ |\lambda_3\mu_3; \alpha_3\rangle_c, \tag{3.63}$$

where R is the operation $\zeta_1 \leftrightarrow \delta_{12}$, $\zeta_3 \leftrightarrow \delta_{34}$, $\zeta_5 \leftrightarrow \delta_{56}$, [see Eq. (2.20)] and $\mathcal{R}$ changes the labels $\lambda_i \leftrightarrow \mu_i$, $\alpha_i \to -\alpha_i$ [see Eq. (2.22b)], and

$$A = \left\{\frac{(\mu_1 + 1)!\,(\mu_2 + 1)!\,(\lambda_3 + 1)!}{(\lambda_1 + 1)!\,(\lambda_2 + 1)!\,(\mu_3 + 1)!}\right\}^{\frac{1}{2}} \tag{3.64}$$

using Eqs. (2.20) and (2.21). From Eq. (3.14) and the fact that $(h_k(\rho_i), h_k'(\rho_i)) = \delta_{kk'}$

$$[\mathcal{R}Rh_k(\rho_i), \mathcal{R}Rh_k'(\rho_i)] = A^2\ \delta_{kk'} \tag{3.65}$$

using also Eq. (3.63). From Eq. (3.65),

$$a_{21}(\rho_i', k_0') = c_{21}(\rho_i; k_0'),$$

where $c_{ki}(\rho_i, k_0')$ are the coefficients of $h_k'(\rho_i)$, $k_0 - k_0' < 0$, with the normalization factored out [similar to Eq. (3.47)]. $\mathcal{R}$ is the exchange of parameters,

$$\rho_1 \leftrightarrow \rho_6, \qquad \rho_2 \leftrightarrow \rho_3, \qquad \rho_4 \leftrightarrow \rho_5. \tag{3.66}$$

In general then, $a_{ij}(\rho_i', k_0') = c_{ij}(\rho_i, k_0')$. Thus,

$$\mathcal{R}Rh_k(\rho_i) = (-1)^k h_k(\rho_i)'A \tag{3.67}$$

$$k_0 - k_0' \geq 0 \qquad k_0 - k_0' < 0$$

The factor A [Eq. (3.64)] renormalizes the $h_k(\rho_i)$.

$$\mathcal{R}Rh_k(\rho_i) = A \sum_{\alpha_1} \begin{Bmatrix} \mu_1\lambda_1 & \mu_2\lambda_2 & \mu_3\lambda_3 \\ -\alpha_1 & -\alpha_2 & -\alpha_3 \end{Bmatrix}_k \times |\lambda_1\mu_1; \alpha_1\rangle\ |\lambda_2\mu_2; \alpha_2\rangle\ |\lambda_3\mu_3; \alpha_3\rangle_c.$$

The result then follows:

$$\begin{Bmatrix} \mu_1\lambda_1 & \mu_2\lambda_2 & \mu_3\lambda_3 \\ -\alpha_1 & -\alpha_2 & -\alpha_3 \end{Bmatrix}_k = (-1)^k \begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_3\mu_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{Bmatrix}_k. \tag{3.68}$$

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APPENDIX A. ORTHONORMALITY OF BASE VECTORS

Since Condon and Shortley[19] have already given the normalization for the $SU(2)$ lowering operator,

$$|\lambda\mu; ytt_0\rangle = \left\{\frac{(2t - r)!}{(2t)!\,r!}\right\}^{\frac{1}{2}} (T_-)^r\ |\lambda\mu; ytt\rangle,$$

it is only necessary to calculate the normalization for the base vector $|\lambda\mu;\ y,\ t,\ t\rangle$. Equation (2.10a) is, with $r = 0$,

$$
\begin{aligned}
&|\lambda\mu;\ ytt\rangle \\
&= N(\lambda\mu;\ ytt)(-1)^q(\xi_1)^p(\sigma_1)^{\lambda-p}(-\delta_{12}^{(2)})^{\mu-q}(\delta_{12}^{(3)})^q \\
&= N(\lambda\mu;\alpha')(-1)^q \\
&\times \sum \binom{q}{b}\binom{\mu-q}{a}(-1)^{a+b}\xi_1^{(1)}\eta_1^{(2)}\sigma_1^{(3)}\xi_2^{(4)}\eta_2^{(5)}\sigma_2^{(6)}, \qquad \text{(A1)}
\end{aligned}
$$

where

$$
\begin{aligned}
(1) &= \mu + p - (a + b), \qquad (2) = b, \\
(3) &= \lambda - p + q, \qquad (4) = a + b, \\
(5) &= q - b, \qquad (6) = \mu - q - a.
\end{aligned}
$$

Take the inner product $(|\lambda\mu;\ y,\ t,\ t\rangle,\ |\lambda'\mu';\ y',\ t',\ t'\rangle)$. Using Eq. (1.2),

$$
\begin{aligned}
&(2) : b = b', \qquad (4) : a = a', \qquad (5) : q = q', \\
&(6) : \mu = \mu', \qquad (1) : p = p', \qquad (3) : \lambda = \lambda',
\end{aligned}
$$

showing orthogonality. The inner product of Eq. (A1) becomes

$$
= N(\lambda\mu;\ ytt)^2(q!)^2[(\mu - q)!]^2 \sum_{a,b} \frac{p!\ b!\ \lambda!\ a!\ q!\ \mu!}{(a!)^2(b!)^2}
$$

and this may be summed (using binomial identities) to be

$$
\begin{aligned}
&= N(\lambda\mu;\ ytt)^2 \\
&\times \frac{p!\ q!\ (\mu-q)!\ (\lambda-p)!\ (\lambda+\mu-q+1)!\ (\mu+p+1)!}{(\mu+p-q+1)!\ (\lambda+1)!}. \qquad \text{(A2)}
\end{aligned}
$$

$N(\lambda\mu;\ ytt)$, as given in Eq. (A2), times the factor $\{(2t - r)!/(2t)!r!\}^{\frac{1}{2}}$, is $N(\lambda\mu;\ \alpha)$, Eq. (2.10b).

APPENDIX B. EVALUATION OF INTEGRALS

A. Normalization of $h(k_i)$ for the nondegenerate case $[\lambda_1 0] \otimes [\lambda_2 \mu_2]$

$$
\begin{aligned}
&h(k_i) = \Delta(k_i) \\
&\times \frac{[\zeta_1\cdot(\zeta_3\times\zeta_5)]^{k_0}(\zeta_3\cdot\delta_{56})^{k_1}(\zeta_1\cdot\delta_{56})^{k_2}(\zeta_5\cdot\delta_{34})^{k_5}(\zeta_1\cdot\delta_{34})^{k_6}}{k_0!\qquad k_1!\qquad k_2!\qquad k_5!\qquad k_6!}.
\end{aligned}
$$

Divide $h(k_i)$ by $\Delta(k_i)$:

$$
f(k_i) \equiv h(k_i)/\Delta(k_i). \qquad \text{(B1)}
$$

Multiply $f(k_i)$ by $\tau_0^{k_0}\tau_1^{k_1}\tau_2^{k_2}\tau_5^{k_5}\tau_6^{k_6}$ and sum k_i

$$
\begin{aligned}
\Phi &\equiv \sum_{k_i} f(k_i) \prod_i \tau_i^{k_i} \\
&= \exp\{\tau_0[\zeta_1\cdot(\zeta_3\times\zeta_5)] + \tau_1(\zeta_3\cdot\delta_{56}) \\
&\quad + \tau_2(\zeta_1\cdot\delta_{56}) + \tau_5(\zeta_5\cdot\delta_{34}) + \tau_6(\zeta_1\cdot\delta_{34}), \qquad \text{(B2)}
\end{aligned}
$$

$$
[\Phi(\tau_i),\ \Phi(\tau_i')] = \sum_{k_i,k'_i} [f(k_i),\ f(k_i')] \prod_i \bar{\tau}_i^{k_i} \prod_j (\tau_j')^{k'_j}. \qquad \text{(B3)}
$$

Integrate Eq. (B3) with respect to ζ_4, ζ_6:

$$
\begin{aligned}
(\Phi,\ \Phi') &= \int \exp\{\overline{(\tau_1\ \delta_{35} + \tau_2\ \delta_{15})} \\
&\quad \cdot(\tau_1'\ \delta_{35} + \tau_2'\ \delta_{15}) + \tau_0'[\zeta_1\cdot(\zeta_3\times\zeta_5)] \\
&\quad + \overline{(\tau_5\ \delta_{53} + \tau_6\ \delta_{13})}\cdot(\tau_5'\ \delta_{53} + \tau_6'\ \delta_{13}) \\
&\quad + \overline{\tau_0[\zeta_1\cdot(\zeta_3\times\zeta_5)]}\}\ d\mu_9, \qquad \text{(B4)}
\end{aligned}
$$

where use has been made of Bargmann's result[1]

$$
[e_a(z),\ f(z)] = f(a), \qquad e_a(z) = \exp(\bar{a}\cdot z). \qquad \text{(B5)}
$$

Perform a change of variables

$$
\tau_2'\zeta_1' = \tau_2'\zeta_1 + \tau_1'\zeta_3, \qquad \tau_5'\zeta_5' = \tau_5'\zeta_5 + \tau_6'\zeta_1,
$$

and a similar change for the complex-conjugate variables. The exponential of Eq. (B4) has the general form

$$
\exp[-\zeta_3\cdot(b\mathbf{1} - c\mathbf{A})\zeta_3 + \bar{a}_1\cdot\zeta_3 + a_2\cdot\bar{\zeta}_3 + C]. \qquad \text{(B6)}
$$

By a translation of ζ_3, Eq. (B6) may be put in the form

$$
\exp[-\zeta_3'\cdot(b\mathbf{1} - c\mathbf{A})\zeta_3' + D], \qquad \text{(B7)}
$$

$$
\text{where } b = 1 + \tau_1'\bar{\tau}_1/\tau_2'\bar{\tau}_2,\ c = \tau_5'\bar{\tau}_5. \qquad \text{(B8)}
$$

$A_{ij} = (\zeta_5\cdot\bar{\zeta}_5)\delta_{ij} - (\bar{\zeta}_5)_i(\zeta_5)_j$, suppressing primes, and D is independent of ζ_3', $\bar{\zeta}_3'$. Equation (B7) may be integrated with respect to ζ_3' using Bargmann's result,

$$
\int \exp(\bar{z}\cdot\mathbf{A}z)\ d\mu_3(z) = [\det(\mathbf{1} - \mathbf{A})]^{-1}, \qquad \text{(B9)}
$$

where $\bar{z}\cdot\mathbf{A}z = \sum_{ij}\bar{z}_iA_{ij}z_j$, and the matrix $\mathbf{1} - \mathbf{A}$ is assumed to have a positive-definite Hermitian part. The integral of (B7) becomes

$$
(\Phi,\ \Phi') = \int \frac{\exp(D)\ d\mu_6(\zeta_1,\ \zeta_5)}{\det(b\mathbf{1} - c\mathbf{A})}, \qquad \text{(B10)}
$$

$$
\det(b\mathbf{1} - c\mathbf{A}) = b(b - c(\zeta_5\cdot\bar{\zeta}_5))^2.
$$

The denominator of (B10) is only a function of $\zeta_5\cdot\bar{\zeta}_5$, so (B10) may be integrated with respect to ζ_1; $\exp(D)$ may be put in the form

$$
\exp[-\bar{\zeta}_1'\cdot(m\mathbf{1} - \mathbf{H})\zeta_1' + E'], \qquad \text{(B11)}
$$

where

$$
m = 1 + \frac{\tau_6'\bar{\tau}_6}{\tau_5'\bar{\tau}_5} - \frac{\tau_1'\bar{\tau}_1}{\tau_2'\bar{\tau}_2}[b - c(\zeta_5\cdot\bar{\zeta}_5)]^{-1}
$$

and

$$H_{ij} = -h(\zeta_5)_i(\bar{\zeta}_5)_j + k[(\zeta_5\cdot\bar{\zeta}_5)\,\delta_{ij} - (\zeta_5)_i(\bar{\zeta}_5)_j],$$

$$h = c/b\,\frac{\tau_1'\bar{\tau}_1}{\tau_2'\bar{\tau}_2}\,[b - c(\zeta_5\cdot\bar{\zeta}_5)]^{-1},$$

$$k = \tau_2'\bar{\tau}_2 + \tau_0'\bar{\tau}_0[b - c(\zeta_5\cdot\bar{\zeta}_5)]^{-1}.$$

The result of integrating (B11) with respect to ζ_1 is

$$(\Phi, \Phi') = \int \frac{\exp(E)\, d\mu_3(\zeta_5)}{b(b - c(\zeta_5\cdot\bar{\zeta}_5))^2 \det(m\mathbf{1} - \mathsf{H})},$$

If

$$(\zeta_5\cdot\bar{\zeta}_5)\left[1 + \frac{\tau_6'\bar{\tau}_6}{\tau_5'\bar{\tau}_5}\,b\right] = \zeta_5'\cdot\bar{\zeta}_5',$$

then (Φ, Φ') may be put in the simple form

$$(\Phi, \Phi') = \int \frac{d\mu_3(\zeta_5')}{\{1 - [(\tau'\cdot\bar{\tau})(\zeta_5'\cdot\bar{\zeta}_5') - d(\zeta_5'\cdot\bar{\zeta}_5')^2]\}^2}, \tag{B12}$$

where

$$\tau'\cdot\bar{\tau} = \tau_0'\bar{\tau}_0 + \tau_1'\bar{\tau}_1 + \tau_2'\bar{\tau}_2 + \tau_5'\bar{\tau}_5 + \tau_6'\bar{\tau}_6,$$

$$d = \tau_2'\bar{\tau}_2\tau_5'\bar{\tau}_5 + \tau_2'\bar{\tau}_2\tau_6'\bar{\tau}_6 + \tau_1'\bar{\tau}_1\tau_6'\bar{\tau}_6.$$

Expand the denominator of (B12):

$$(\Phi, \Phi') = \sum \frac{(n+1)!\,(-1)^m(\tau'\cdot\bar{\tau})^{n-m}\,d^m}{m!\,(n-m)!}\,I(n+m), \tag{B13}$$

$$I(n+m) = \int d\mu_3(\zeta_5')(\zeta_5'\cdot\bar{\zeta}_5')^{n+m} = \tfrac{1}{2}(n+m+2)! \tag{B14}$$

using (1.2). Thus,

$$(\Phi, \Phi') = \frac{1}{2}\sum \frac{(P+2)!\,(\bar{\tau}_0\tau_0')^{k_0}\cdots(\bar{\tau}_6\tau_6')^{k_6}}{k_0!}\,S,$$

where $P = k_0 + k_1 + k_2 + k_5 + k_6$ and

$$S = \sum \frac{(P+1-m)!\,(-1)^m}{(k_1 - m + y_1 + y_2)!\,(k_2 - y_1 - y_2)!\,(k_5 - y_1)!\,(k_6 - m + y_1)!\,y_1!\,y_2!\,(m - y_1 - y_2)!}.$$

S may be summed using binomial identities, and the result is

$$(\Phi, \Phi') = \frac{1}{2}\sum \frac{(\tau_0'\bar{\tau}_0)^{k_0}\cdots(\tau_6'\bar{\tau}_6)^{k_6}(P+2)!}{k_0!\,k_1!\,k_2!\,k_5!\,k_6!} \times \frac{(k_0+k_5+k_6+1)!\,(k_0+k_1+k_2+1)!\,(k_0+k_1+k_4+1)!}{(k_0+k_1+1)!\,(k_0+k_5+1)!}. \tag{B15}$$

Comparison of (B15) and (B3) provides Eq. (3.23).

The expansion of the denominator of (B12), and similar expansions in this Appendix, may be justified in the following manner. In Eq. (B3), let $J(k_i, k_j') = [f(k_i), f(k_j')]$ be written $J(A; k_i, k_j')$, where the integration of ζ_5 is not taken over the entire plane, but only over a finite portion.

$$J(k_i, k_j') = \lim_{A\to\infty} J(A; k_i, k_j').$$

The integral (B12) would be written

$$(\Phi, \Phi') = \int_A \frac{d\mu_3(\zeta_5)}{\{1 - [\tau'\cdot\bar{\tau})(\zeta_5\cdot\bar{\zeta}_5) - d(\zeta_5\cdot\bar{\zeta}_5)^2]\}^2}.$$

This integral may be expanded, since the τ's may be made sufficiently small. The coefficient of $\prod(\bar{\tau}_i)^{k_i}\prod\tau'^{k_j}_j$ is $J(A; k_i, k_j')$, or

$$(\Phi, \Phi') = \sum \frac{(n+1)!\,(-1)^m(\tau'\cdot\bar{\tau})^{n-m}\,d^m}{m!\,(n-m)!} \times I(A, n+m),$$

$$I(A, n+m) = \int_A d\mu_3(\zeta_5)(\zeta_5\cdot\bar{\zeta}_5)^{n+m}.$$

In this integral, the limit may be taken,

$$I(n+m) \equiv \lim_{A\to\infty} I(A, n+m) = \tfrac{1}{2}(n+m+2)!$$

The integral (B12), and similar types, are well defined if they are understood in the above sense.

B. Normalization for $h_k(\rho_i)$

In order to calculate the normalization for $h_k(\rho_j)$,

$$h_k(\rho_j) = \sum_{m_1+m_2=N} \beta_k(\rho_j; n_1, n_2)H(k_i),$$

where

$$H(k_i) = [\zeta_1\cdot(\zeta_3\times\zeta_5)]^{k_0}F(\rho_i)H_1^{n_1}(H_2)^{n_2}$$

and $F(\rho_i)$ is given by Eq. (3.28b), with

$$k_i = \rho_i + n_1, \qquad k_i' = \rho_i' + n_1', \qquad i = 1, 3, 5,$$

$$k_i = \rho_i + n_2, \qquad k_i' = \rho_i' + n_2', \qquad i = 2, 4, 6,$$

it is necessary to evaluate the inner product $[H(k_i), H(k_i')]$. Multiply $H(k_i)$ by $\prod(\tau_i^{k_i}/k_i'!)$ and sum over k_i:

$$(\Phi, \Phi') = \sum_{k_i, k_j'} [H(k_i), H(k_j')] \times \prod \left(\frac{(\bar{\tau}_i)^{k_i}}{k_i!}\right) \prod \left(\frac{(\tau_j')^{k_j'}}{k_j'!}\right) \quad \text{(B16)}$$

$$= \int \exp [\Phi(\bar{\tau}_i, \bar{\zeta}) + \Phi(\tau_j', \zeta)]\, d\mu_{18}(\zeta). \quad \text{(B17)}$$

The integration may first be performed with respect to ζ_2, ζ_4, ζ_6, using Eq. (B5), and then ζ_5, using Eq. (B9). The result may then be expanded and integrated with respect to the remaining variables. The sums may be contracted by means of binomial identities. The following result is obtained:

$$(\Phi, \Phi') = \sum (\bar{\tau}_0\tau_0')^{k_0}\beta^{\alpha_3}(-d)^{\alpha_3}[(4) + (6)]^{\alpha_1}[(3)(4)]^{z_4} \times [(2) + (3)]^{z_4}[(5)(6)]^{z_5}[(1) + (5)]^{z_6} \cdot S, \quad \text{(B18)}$$

where $(i) = \bar{\tau}_i\tau_i'$ (no summation) and S is the factor

$$S = \frac{(m_1 + k_0 + \alpha_2 + 1)!\,(2m_1 + 2k_0 + 2\alpha_2 + \alpha_3 - \alpha_1 + z_4 + z_6 + 3)!}{k_0!\,2z_3!\,z_4!\,z_5!\,z_6!\,\alpha_1!\,(m_1 + k_0 + \alpha_2 - \alpha_1 + 1)!\,\alpha_2!\,\alpha_3!} \times \frac{(2m_1 + k_0 + 2\alpha_2 - \alpha_1 + z_4 + z_6 + 2)!\,(m_1 + k_0 + \alpha_2 - \alpha_1 + z_4 + z_6 + 1)!}{(2m_1 + 2k_0 + 2\alpha_2 - \alpha_1 + z_4 + z_6 + 3)!}, \quad \text{(B19)}$$

$$m_1 = z_3 + z_5 + \alpha_1 + \alpha_3, \quad \text{(B20)}$$

$$d = (1)(3) + (2)(5) + (3)(5) = \overline{(\tau_1\tau_3\tau_5 - \tau_2\tau_4\tau_6)}(\tau_1'\tau_3'\tau_5' - \tau_2'\tau_4'\tau_6').$$

Expression (B18) must now be expanded out. The terms may be collected in the form:

$$(0)^{k_0}(1)^{\rho_1}\cdots(6)^{\rho_6}\overline{(\tau_1\tau_3\tau_5)}^{x_1}\overline{(\tau_2\tau_4\tau_6)}^{x_2}(\tau_1'\tau_3'\tau_5')^{y_1}(\tau_2'\tau_4'\tau_6')^{y_2},$$

where $x_1 + x_2 = N = y_1 + y_2$

with the appropriate coefficient giving the result $[H(k_i), H(k_j')]$.

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Recoupling Coefficients for the Group $SU(3)$*

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The Hilbert space method, employed in the previous article to obtain the coupling coefficients of $SU(3)$, is used here to obtain the recoupling, or $6(\lambda\mu)$, coefficients of $SU(3)$. The coefficients are formulated in terms of a generating function involving an integral, and an explicit expression is integrated out for the general nondegenerate case. The symmetries of the $6(\lambda\mu)$ coefficients are discussed.

1. INTRODUCTION

THE $6(\lambda\mu)$ coefficient of $SU(3)$, which relates the alternate ways three representations $[\lambda_i, \mu_i]$, $i = 1, 2, 3$, may be coupled, can be written in the form[1]

$$\begin{bmatrix} \lambda\mu; k, k' & \lambda_2\mu_2 & \lambda_{12}\mu_{12}; k_{12} \\ \lambda_1\mu_1 & \lambda_3\mu_3 & \lambda_{13}\mu_{13}; k_{13} \end{bmatrix} = \sum_{\alpha_i} \begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_{12}\mu_{12} \\ \alpha_1 & \alpha_2 & \alpha_{12} \end{Bmatrix}_{k_{12}} \begin{Bmatrix} \lambda_{12}\mu_{12} & \lambda_3\mu_3 & \lambda\mu \\ \alpha_{12} & \alpha_3 & \alpha \end{Bmatrix}_{k} \times \begin{Bmatrix} \mu_{13}\lambda_{13} & \mu_2\lambda_2 & \mu\lambda \\ -\alpha_{13} & -\alpha_2 & -\alpha \end{Bmatrix}_{k'} \begin{Bmatrix} \mu_1\lambda_1 & \mu_3\lambda_3 & \mu_{13}\lambda_{13} \\ -\alpha_1 & -\alpha_3 & -\alpha_{13} \end{Bmatrix}_{k_{13}}, \quad (1.1)$$

where use has been made of the orthogonal properties[2] and the symmetry properties of the $3(\lambda\mu)$ coefficients derived in the previous paper.[3]

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[1] A form similar to this has been derived by J. J. de Swart, Nuovo Cimento 31, 420 (1964). Equation (1.1) is the recoupling coefficient multiplied by the factor $(-1)^{k'+k_{13}}(N_{12}N_{13})^{-1/2}$, where N_{12} and N_{13} are the dimensions of the spaces

$$\mathfrak{D}_{\lambda_{12}\mu_{12}}, \mathfrak{D}_{\lambda_{13},\mu_{13}}$$

(see Ref. 3 below).

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

[3] M. Resnikoff, preceding paper, J. Math. Phys. 8, 63 (1967). This article is hereafter referred to as (I).

$$(\Phi, \Phi') = \sum_{k_i, k_j'} [H(k_i), H(k_j')] \times \prod \left(\frac{(\bar{\tau}_i)^{k_i}}{k_i!}\right) \prod \left(\frac{(\tau_j')^{k_j'}}{k_j'!}\right) \quad \text{(B16)}$$

$$= \int \exp [\Phi(\bar{\tau}_i, \bar{\zeta}) + \Phi(\tau_j', \zeta)]\, d\mu_{18}(\zeta). \quad \text{(B17)}$$

The integration may first be performed with respect to ζ_2, ζ_4, ζ_6, using Eq. (B5), and then ζ_5, using Eq. (B9). The result may then be expanded and integrated with respect to the remaining variables. The sums may be contracted by means of binomial identities. The following result is obtained:

$$(\Phi, \Phi') = \sum (\bar{\tau}_0\tau_0')^{k_0}\beta^{\alpha_3}(-d)^{\alpha_3}[(4) + (6)]^{\alpha_1}[(3)(4)]^{z_4} \times [(2) + (3)]^{z_4}[(5)(6)]^{z_5}[(1) + (5)]^{z_6} \cdot S, \quad \text{(B18)}$$

where $(i) = \bar{\tau}_i\tau_i'$ (no summation) and S is the factor

$$S = \frac{(m_1 + k_0 + \alpha_2 + 1)!\,(2m_1 + 2k_0 + 2\alpha_2 + \alpha_3 - \alpha_1 + z_4 + z_6 + 3)!}{k_0!\,2z_3!\,z_4!\,z_5!\,z_6!\,\alpha_1!\,(m_1 + k_0 + \alpha_2 - \alpha_1 + 1)!\,\alpha_2!\,\alpha_3!} \times \frac{(2m_1 + k_0 + 2\alpha_2 - \alpha_1 + z_4 + z_6 + 2)!\,(m_1 + k_0 + \alpha_2 - \alpha_1 + z_4 + z_6 + 1)!}{(2m_1 + 2k_0 + 2\alpha_2 - \alpha_1 + z_4 + z_6 + 3)!}, \quad \text{(B19)}$$

$$m_1 = z_3 + z_5 + \alpha_1 + \alpha_3, \quad \text{(B20)}$$

$$d = (1)(3) + (2)(5) + (3)(5) = \overline{(\tau_1\tau_3\tau_5 - \tau_2\tau_4\tau_6)}(\tau_1'\tau_3'\tau_5' - \tau_2'\tau_4'\tau_6').$$

Expression (B18) must now be expanded out. The terms may be collected in the form:

$$(0)^{k_0}(1)^{\rho_1}\cdots(6)^{\rho_6}\overline{(\tau_1\tau_3\tau_5)}^{x_1}\overline{(\tau_2\tau_4\tau_6)}^{x_2}(\tau_1'\tau_3'\tau_5')^{y_1}(\tau_2'\tau_4'\tau_6')^{y_2},$$

where $x_1 + x_2 = N = y_1 + y_2$

with the appropriate coefficient giving the result $[H(k_i), H(k_j')]$.

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Recoupling Coefficients for the Group $SU(3)$*

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The Hilbert space method, employed in the previous article to obtain the coupling coefficients of $SU(3)$, is used here to obtain the recoupling, or $6(\lambda\mu)$, coefficients of $SU(3)$. The coefficients are formulated in terms of a generating function involving an integral, and an explicit expression is integrated out for the general nondegenerate case. The symmetries of the $6(\lambda\mu)$ coefficients are discussed.

1. INTRODUCTION

THE $6(\lambda\mu)$ coefficient of $SU(3)$, which relates the alternate ways three representations $[\lambda_i, \mu_i]$, $i = 1, 2, 3$, may be coupled, can be written in the form[1]

$$\begin{bmatrix} \lambda\mu; k, k' & \lambda_2\mu_2 & \lambda_{12}\mu_{12}; k_{12} \\ \lambda_1\mu_1 & \lambda_3\mu_3 & \lambda_{13}\mu_{13}; k_{13} \end{bmatrix} = \sum_{\alpha_i} \begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_{12}\mu_{12} \\ \alpha_1 & \alpha_2 & \alpha_{12} \end{Bmatrix}_{k_{12}} \begin{Bmatrix} \lambda_{12}\mu_{12} & \lambda_3\mu_3 & \lambda\mu \\ \alpha_{12} & \alpha_3 & \alpha \end{Bmatrix}_{k} \times \begin{Bmatrix} \mu_{13}\lambda_{13} & \mu_2\lambda_2 & \mu\lambda \\ -\alpha_{13} & -\alpha_2 & -\alpha \end{Bmatrix}_{k'} \begin{Bmatrix} \mu_1\lambda_1 & \mu_3\lambda_3 & \mu_{13}\lambda_{13} \\ -\alpha_1 & -\alpha_3 & -\alpha_{13} \end{Bmatrix}_{k_{13}}, \quad (1.1)$$

where use has been made of the orthogonal properties[2] and the symmetry properties of the $3(\lambda\mu)$ coefficients derived in the previous paper.[3]

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[1] A form similar to this has been derived by J. J. de Swart, Nuovo Cimento 31, 420 (1964). Equation (1.1) is the recoupling coefficient multiplied by the factor $(-1)^{k'+k_{13}}(N_{12}N_{13})^{-1/2}$, where N_{12} and N_{13} are the dimensions of the spaces

$$\mathfrak{D}_{\lambda_{12}\mu_{12}}, \mathfrak{D}_{\lambda_{13},\mu_{13}}$$

(see Ref. 3 below).

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

[3] M. Resnikoff, preceding paper, J. Math. Phys. 8, 63 (1967). This article is hereafter referred to as (I).

2. SYMMETRY OF THE 6($\lambda\mu$) COEFFICIENTS

From the symmetries of the 3($\lambda\mu$) coefficients[4] [see Sec. 3D. of (I)], many symmetries of the 6($\lambda\mu$) coefficients are apparent from Eq. (1.1).

Exchange of columns 1, 2

Let

$$\lambda_1\mu_1 \leftrightarrow \mu_3\lambda_3, \quad \lambda\mu \leftrightarrow \lambda_2\mu_2, \quad \lambda_{13}\mu_{13} \leftrightarrow \mu_{13}\lambda_{13} \tag{2.1a}$$

be exchanged and let $k \leftrightarrow k_{12}$ also be exchanged in Eq. (1.1). The right-hand side of Eq. (1.1) becomes

$$\sum_{\alpha_i} \begin{Bmatrix} \mu_3\lambda_3 & \lambda\mu & \lambda_{12}\mu_{12} \\ -\alpha_3 & \alpha & \alpha_{12} \end{Bmatrix}_k \begin{Bmatrix} \lambda_{12}\mu_{12} & \mu_1\lambda_1 & \lambda_2\mu_2 \\ \alpha_{12} & -\alpha_1 & \alpha_2 \end{Bmatrix}_{k_{12}} \times \begin{Bmatrix} \lambda_{13}\mu_{13} & \lambda\mu & \lambda_2\mu_2 \\ \alpha_{13} & \alpha & \alpha_2 \end{Bmatrix}_{k'} \begin{Bmatrix} \lambda_3\mu_3 & \lambda_1\mu_1 & \lambda_{13}\mu_{13} \\ \alpha_3 & \alpha_1 & \alpha_{13} \end{Bmatrix}_{k_{13}}. \tag{2.1b}$$

The right-hand side of Eq. (2.1b) is equal to the right-hand side of Eq. (1.1) [using Eqs. (3.56), (3.59), (3.61), (3.68) of (I)], except for a phase. The result follows that

$$\begin{bmatrix} \lambda\mu; k, k' & \lambda_2\mu_2 & \lambda_{12}\mu_{12}; k_{12} \\ \lambda_1\mu_1 & \lambda_3\mu_3 & \lambda_{13}\mu_{13}; k_{13} \end{bmatrix} = (-1)^A \begin{bmatrix} \lambda_2\mu_2; k_{12}k' & \lambda\mu & \lambda_{12}\mu_{12}; k \\ \mu_3\lambda_3 & \mu_1\lambda_1 & \mu_{13}\lambda_{13}; k_{13} \end{bmatrix}, \tag{2.1c}$$

where

$$A = \lambda_1 + \lambda_3 + \lambda + \mu_2 - (\mu + \mu_1 + \mu_3 + \lambda_2) + k + k_{12}.$$

The other relations follow similarly.

Exchange of columns 1, 3

Let

$$\lambda_1\mu_1 \leftrightarrow \mu_{13}\lambda_{13}, \quad \lambda\mu \leftrightarrow \mu_{12}\lambda_{12}, \quad \lambda_2\mu_2 \leftrightarrow \mu_2\lambda_2, \tag{2.2a}$$

and $k_{12} \leftrightarrow k'$, be exchanged. Then

$$\begin{bmatrix} \lambda\mu; k,k' & \lambda_2\mu_2 & \lambda_{12}\mu_{12}; k_{12} \\ \lambda_1\mu_1 & \lambda_3\mu_3 & \lambda_{13}\mu_{13}; k_{13} \end{bmatrix} = (-1)^B \begin{bmatrix} \mu_{12}\lambda_{12}; k,k_{12} & \mu_2\lambda_2 & \mu\lambda; k' \\ \mu_{13}\lambda_{13} & \lambda_3\mu_3 & \mu_1\lambda_1; k_{13} \end{bmatrix}, \tag{2.2b}$$

where

$$B = \mu + \mu_1 + \lambda_2 + \lambda_{13} - (\lambda + \mu_{12} + \mu_{13} + \lambda_1) + k + k_{13}.$$

These symmetries relate six of the 6($\lambda\mu$) symbols.

[4] J. R. Derome and W. T. Sharp, J. Math. Phys. **6**, 1584 (1965), have discussed symmetries for the 6-j symbols of a general group. In contrast to their paper, the phase and the method of labeling degenerate states is specified here, and this leads to simpler relations. de Swart (Ref. 1) obtains symmetry relations for octet recouplings.

Inversion of columns 1, 2

Let

$$\lambda_1\mu_1 \leftrightarrow \lambda\mu, \quad \lambda_2\mu_2 \leftrightarrow \mu_3\lambda_3, \tag{2.3a}$$

and $k_{12} \leftrightarrow k$, $k_{13} \leftrightarrow k'$, be exchanged. Then

$$\begin{bmatrix} \lambda\mu; k,k' & \lambda_2\mu_2 & \lambda_{12}\mu_{12}; k_{12} \\ \lambda_1\mu_1 & \lambda_3\mu_3 & \lambda_{13}\mu_{13}; k_{13} \end{bmatrix} = \begin{bmatrix} \lambda_1\mu_1; k_{12},k_{13} & \mu_3\lambda_3 & \lambda_{12}\mu_{12}; k \\ \lambda\mu & \mu_2\lambda_2 & \lambda_{13}\mu_{13}; k' \end{bmatrix}. \tag{2.3b}$$

Inversion of columns 1, 3

Let

$$\lambda\mu \leftrightarrow \mu_1\lambda_1, \quad \lambda_{12}\mu_{12} \leftrightarrow \mu_{13}\lambda_{13} \tag{2.4a}$$

and $k_{12} \leftrightarrow k'$, $k_{13} \leftrightarrow k$, be exchanged. Then,

$$\begin{bmatrix} \lambda\mu; k,k' & \lambda_2\mu_2 & \lambda_{12}\mu_{12}; k_{12} \\ \lambda_1\mu_1 & \lambda_3\mu_3 & \lambda_{13}\mu_{13}; k_{13} \end{bmatrix} = \begin{bmatrix} \mu_1\lambda_1; k_{13},k_{12} & \lambda_2\mu_2 & \mu_{13}\lambda_{13}; k' \\ \mu\lambda & \lambda_3\mu_3 & \mu_{12}\lambda_{12}; k \end{bmatrix}. \tag{2.4b}$$

Finally, if the partition numbers are exchanged, $\lambda_i \leftrightarrow \mu_i$, then the right-hand side of Eq. (1.1) is a sum over conjugate 3($\lambda\mu$) symbols, and the symmetry relation, Eq. (3.68) of (I), may be employed, with the result

$$\begin{bmatrix} \lambda\mu; k,k' & \lambda_2\mu_2 & \lambda_{12}\mu_{12}; k_{12} \\ \lambda_1\mu_1 & \lambda_3\mu_3 & \lambda_{13}\mu_{13}; k_{13} \end{bmatrix} = (-1)^C \begin{bmatrix} \mu\lambda; k,k' & \mu_2\lambda_2 & \mu_{12}\lambda_{12}; k_{12} \\ \mu_1\lambda_1 & \mu_3\lambda_3 & \mu_{13}\lambda_{13}; k_{13} \end{bmatrix}, \tag{2.5}$$

where

$$C = k + k + k_{12} + k_{13}.$$

This symmetry is present in $SU(3)$ because the base vector $|\lambda\mu;\ \alpha\rangle$ and the conjugate base vector $|\lambda\mu;\ \alpha\rangle_c$ are in different Hilbert spaces. In $SU(2)$, v_m^j and w_m^j are members of the same Hilbert space.[5] The 3 $-$ j symbol

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

and its conjugate

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}$$

are related by a phase, but since the spaces, labeled by j, are the same, a change to the conjugate 6 $-$ j symbol yields no further relations. In general, then, 48 6($\lambda\mu$) coefficients are related by a phase.

[5] V. Bargmann, Rev. Mod. Phys. **34**, 829 (1962).

3. 6(λμ) COEFFICIENT EXPRESSED AS AN INTEGRAL

Notation: Let the variables of the base vector $|\lambda\mu;\ \alpha\rangle$ be written $f(\zeta,\ \zeta')$ or $f(\zeta,\ \delta)$, and the base vector with complex conjugate variables $\bar{\zeta},\ \bar{\delta}$ be written $\overline{|\lambda\mu;\ \alpha\rangle}$. Also, let the invariants $h_k(\rho_i)$ be written $h_k(\zeta_1,\ \delta_1;\ \zeta_2,\ \delta_2;\ \zeta_3,\ \delta_3)$, where the explicit functional dependence is exhibited.[6]

The variables of the invariants $h_k(\rho_i)$ are chosen such that a product of four $h_k(\rho_i)$, integrated over the variables ζ_i, yields a multiple of the 6(λμ) coefficient, as given by Eq. (1.1). First, associate, with each 3(λμ) coefficient appearing in Eq. (1.1) an appropriate invariant $h_j(\rho_i)$, $j = 1, \ldots, 4$:

$$h_1 \equiv h_{k_{12}}(\zeta_1,\ \delta_1;\ \zeta_2,\ \delta_2;\ \zeta_{12},\ \delta_{12})$$
$$= \sum_{\alpha_1\alpha_2\alpha_{12}} \begin{Bmatrix} \lambda_1\mu_1 & \lambda_2\mu_2 & \lambda_{12}\mu_{12} \\ \alpha_1 & \alpha_2 & \alpha_{12} \end{Bmatrix}_{k_{12}}$$
$$\times\ |\lambda_1\mu_1;\ \alpha_1\rangle\ |\lambda_2\mu_2;\ \alpha_2\rangle\ |\lambda_{12}\mu_{12};\ \alpha_{12}\rangle_c. \qquad (3.1a)$$

In

$$h_k(\zeta_{12},\ \delta_{12};\ \zeta_3,\ \delta_3;\ \zeta,\ \delta) = \sum_{\alpha_{12}',\alpha_3,\alpha} \begin{Bmatrix} \lambda_{12}\mu_{12} & \lambda_3\mu_3 & \lambda\mu \\ \alpha_{12}' & \alpha_3 & \alpha \end{Bmatrix}_k$$
$$\times\ |\lambda_{12}\mu_{12};\ \alpha_{12}'\rangle\ |\lambda_3\mu_3;\ \alpha_3\rangle\ |\lambda\mu;\ \alpha\rangle_c,$$

exchange $\zeta_{12} \leftrightarrow \delta_{12}$, $\zeta \leftrightarrow \delta$, and complex conjugate these variables to get

$$h_2 \equiv h_k(\bar{\delta}_{12},\ \bar{\zeta}_{12};\ \zeta_3,\ \delta_3;\ \bar{\delta},\ \bar{\zeta})$$
$$= \sum_{\alpha_{12}'\alpha_3\alpha} \begin{Bmatrix} \lambda_{12}\mu_{12} & \lambda_3\mu_3 & \lambda\mu \\ \alpha_{12}' & \alpha_3 & \alpha \end{Bmatrix}_k \left\{\frac{(\lambda_{12}+1)!\,(\mu+1)!}{(\mu_{12}+1)!\,(\lambda+1)!}\right\}^{\frac{1}{2}}$$
$$\times\ \overline{|\lambda_{12}\mu_{12};\ \alpha_{12}\rangle}_c\ |\lambda_3\mu_3;\ \alpha_3\rangle\ \overline{|\lambda\mu;\ \alpha\rangle}. \qquad (3.1b)$$

The degree conditions [see Sec. 3C of (I)] are chosen [Eq. (3.6)] such that the 3(λμ) coefficient appearing in Eq. (1.1) is obtained. Similarly,

$$h_3 \equiv h_{k'}(\bar{\delta}_{13},\ \bar{\zeta}_{13};\ \bar{\delta}_2,\ \bar{\zeta}_2;\ \zeta,\ \delta)$$
$$= \sum_{\alpha'\alpha_2'\alpha_{13}'} \begin{Bmatrix} \mu_{13}\lambda_{13} & \mu_2\lambda_2 & \mu\lambda \\ -\alpha_{13}' & -\alpha_2' & -\alpha' \end{Bmatrix}_{k'}$$
$$\times \left\{\frac{(\mu_2+1)!\,(\mu_{13}+1)!}{(\lambda_2+1)!\,(\lambda_{13}+1)!}\right\}^{\frac{1}{2}}$$
$$\times\ \overline{|\lambda_{13}\mu_{13};\ \alpha_{13}'\rangle}\ \overline{|\lambda_2\mu_2;\ \alpha_2'\rangle}\ |\lambda\mu;\ \alpha'\rangle \qquad (3.1c)$$

and

$$h_4 \equiv h_{k_{13}}(\bar{\delta}_1,\ \bar{\zeta}_1;\ \bar{\delta}_3,\ \bar{\zeta}_3;\ \zeta_{13},\ \delta_{13})$$
$$= \sum_{\alpha_1'\alpha_3'\alpha_{13}'} \begin{Bmatrix} \mu_1\lambda_1 & \mu_3\lambda_3 & \mu_{13}\lambda_{13} \\ -\alpha_1' & -\alpha_3' & -\alpha_{13} \end{Bmatrix}_{k_{13}}$$
$$\times \left\{\frac{(\mu_1+1)!\,(\mu_3+1)!}{(\lambda_1+1)!\,(\lambda_3+1)!}\right\}^{\frac{1}{2}}$$
$$\times\ \overline{|\lambda_1\mu_1;\ \alpha_1'\rangle}\ \overline{|\lambda_3\mu_3;\ \alpha_3'\rangle}\ |\lambda_{13}\mu_{13};\ \alpha_{13}\rangle. \qquad (3.1d)$$

The variables of the four invariants, Eqs. (3.1), have been exchanged such that the functions $h_j(\rho_i)$ are still invariants in the triple product space. Further, for each base vector $|\lambda\mu;\ \alpha\rangle$, there exists the corresponding base vector $\overline{|\lambda\mu;\ \alpha'\rangle}$ with complex conjugate variables. An integral over the product of invariants then yields the inner products, $(|\lambda\mu;\ \alpha'\rangle,\ |\lambda\mu;\ \alpha\rangle) = \delta_{\alpha,\alpha'}$, since the base vectors $|\lambda\mu;\ \alpha\rangle$ are orthonormal [see Eq. (2.9) of (I)]. If the degree conditions are chosen to give the 3(λμ) coefficients of Eqs. (3.1), then the product of the four $h_j(\rho_i)$, integrated over ζ_i, should give, within factors $A_i = [(\mu_i+1)!/(\lambda_i+1)!]^{\frac{1}{2}}$, the 6(λμ) coefficient on the right-hand side of Eq. (1.1). Thus[7]

$$\int \prod_{j=1}^{4} h_j(\rho_i)\ d\mu_{36}(\zeta) = C[6(\lambda\mu)], \qquad (3.2)$$

where

$$C = \left\{\frac{(\lambda_{12}+1)!\,(\mu+1)!\,(\lambda_2+1)!\,(\mu_{13}+1)!\,(\mu_1+1)!\,(\mu_3+1)!}{(\mu_{12}+1)!\,(\lambda+1)!\,(\mu_2+1)!\,(\lambda_{13}+1)!\,(\lambda_1+1)!\,(\lambda_3+1)!}\right\}^{\frac{1}{2}}.$$

The factor C arises because the exchange of variables $\zeta \leftrightarrow \delta$ changes the normalization of the base vector [see Eq. (2.21) of (I)]. As seen in Sec. 3D of (I), it also changes the normalization of the invariant $h_k(\rho_i)$ by the same factor. If the four $h_j(\rho_i)$ are assumed normalized before the appropriate change in variables, factor C may be dropped. That is, if

$$[h_1(\zeta_1,\ \delta_1;\ \zeta_2,\ \delta_2;\ \zeta_{12},\ \delta_{12}),\ h_1(\zeta_1,\ \delta_1;\ \zeta_2,\ \cdots)] = 1 \qquad (3.3)$$

(and similarly for h_2, h_3, h_4), then Eq. (3.2) may be written as

$$\int \prod_{j=1}^{4} h_j(\rho_i)\ d\mu_{36}(\zeta) = [6(\lambda\mu)]. \qquad (3.4)$$

Let ρ_{ij} be the power of the determinants,[6] where $i = 1, 2, 3, 4$ labels the particular invariant $h_j(\zeta)$, [Eq. (3.1)] and $j = 0, 1, \cdots, 6, 0'$ labels the determinant. Let κ_{ij}, $i = 1, \cdots, 4$, $j = 1, \cdots, 6$, be the partition numbers,

[6] The general functional dependence is given by Eqs. (3.33), (3.34), and (3.35) of (I).

[7] The measure $d\mu_n(\zeta)$ is defined in Eq. (1.1b) of (I), or see Bargmann (Ref. 5).

$$\kappa_{1j} = (\mu_{12}, \lambda_2, \lambda_1, \lambda_{12}, \mu_2, \mu_1), \tag{3.5a}$$

$$\kappa_{2j} = (\mu, \lambda_3, \lambda_{12}, \lambda, \mu_3, \mu_{12}), \tag{3.5b}$$

$$\kappa_{3j} = (\lambda, \mu_2, \mu_{13}, \mu, \lambda_2, \lambda_{13}), \tag{3.5c}$$

$$\kappa_{4j} = (\lambda_{13}, \mu_3, \mu_1, \mu_{13}, \lambda_3, \lambda_1). \tag{3.5d}$$

The degree conditions become

$$\begin{aligned} k_{i0} + \rho_{i3} + \rho_{i6} + N_i &= \kappa_{i1}, \\ k_{i0} + \rho_{i1} + \rho_{i4} + N_i &= \kappa_{i2}, \\ k_{i0} + \rho_{i2} + \rho_{i5} + N_i &= \kappa_{i3}, \\ k'_{i0} + \rho_{i1} + \rho_{i2} + N_i &= \kappa_{i4}, \\ k'_{i0} + \rho_{i5} + \rho_{i6} + N_i &= \kappa_{i5}, \\ k'_{i0} + \rho_{i3} + \rho_{i4} + N_i &= \kappa_{i6}, \end{aligned} \qquad \rho_{ij} \geq 0 \tag{3.6}$$

and

$$\begin{aligned} k_{i0} - k'_{i0} &= P_i - (\kappa_{i4} + \kappa_{i5} + \kappa_{i6}), \\ P_i &= \tfrac{1}{3}[\kappa_{i1} + \kappa_{i2} + \kappa_{i3} + 2(\kappa_{i4} + \kappa_{i5} + \kappa_{i6})]. \end{aligned} \tag{3.7}$$

The ρ_{ij} of Eq. (3.6) are not independent, e.g., μ_{12} occurs in Eq. (3.5a) and (3.5b), so that relation $k_{10} + \rho_{13} + \rho_{16} + N_1 = k'_{20} + \rho_{23} + \rho_{24} + N_2$ holds. There are 11 other such relations called by Bargmann[5] the compatibility conditions. Note in the above that either k_{i0} or k'_{i0} is equal to zero, depending on whether $k_{i0} - k'_{i0}$ is ≥ 0 or < 0, respectively [see Eq. (3.32) of (I)].

If the explicit form of $h_i(\rho_{ij})$ is inserted in Eq. (3.4), then

$$[6(\lambda\mu)] = \sum_{n_{i1}+n_{i2}=N_i} \prod_{m=1}^{4} \beta_{km}(\rho_{mj}; n_{m1}, n_{m2}) I(k_{ij}), \tag{3.8}$$

where

$$I(k_{ij}) = \int \prod_{m=1}^{4} (H_{m1})^{n_{m1}} (H_{m2})^{n_{m2}} \times F(\rho_{mj}) G^{(m)}(k_{m0}, k'_{m0})\, d\mu_{36}(\zeta) \tag{3.9}$$

and $G^{(m)}(k_{m0}, k'_{m0})$ represents the determinants raised to the k_{m0} or k'_{m0} power, e.g., in $h_1(\rho_{ij})$,

$$G^1(k_{10}, 0) = [(\zeta_1 \times \zeta_2)\cdot\zeta_{12}]^{k_{10}}, \qquad k_{10} - k'_{10} \geq 0.$$

To obtain the $6(\lambda\mu)$ coefficients, it would be necessary to integrate Eq. (3.9). This integral may be evaluated, but it would involve numerous sums over a product of factorials. There is no particular utility in presenting it here since, if particular numbers are required, Eqs. (3.8), (3.9), may be programmed. A particularly simple case, the nondegenerate case, is carried out in the next section.

4. $6(\lambda\mu)$ SYMBOL FOR THE NONDEGENERATE CASE

Let $\mu_1, \mu_2, \mu_3 = 0$. The $6(\lambda\mu)$ symbol becomes

$$[6(\lambda\mu)] = \begin{bmatrix} \lambda\mu & \lambda_2 0 & \lambda_{12}\mu_{12} \\ \lambda_1 0 & \lambda_3 0 & \lambda_{13}\mu_{13} \end{bmatrix}. \tag{4.1}$$

According to Eqs. (3.6), the invariants $h_i(\rho_{ij})$ are

$$h_1 = \Delta_1 \frac{[(\zeta_1 \times \zeta_2)\cdot\zeta_{12}]^{k_{10}} (\zeta_2\cdot\delta_{12})^{\rho_{11}} (\zeta_1\cdot\delta_{12})^{\rho_{12}}}{k_{10}!\qquad \rho_{11}!\qquad \rho_{12}!}, \tag{4.2a}$$

$$h_2 = \Delta_2 \frac{[\bar\delta_{12}\cdot(\zeta_3 \times \bar\delta)]^{k_{20}} (\zeta_3\cdot\bar\zeta)^{\rho_{21}} (\bar\zeta\cdot\bar\delta_{12})^{\rho_{22}} (\bar\zeta_{12}\cdot\bar\delta)^{\rho_{23}} (\zeta_3\cdot\bar\zeta_{12})^{\rho_{24}}}{k_{20}!\qquad \rho_{21}!\qquad \rho_{22}!\qquad \rho_{23}!\qquad \rho_{24}!}, \tag{4.2b}$$

$$h_3 = \Delta_3 \frac{(\zeta\cdot\bar\zeta_{13})^{\rho_{33}} (\bar\delta_{13}\cdot\delta)^{\rho_{32}} (\zeta\cdot\bar\zeta_2)^{\rho_{36}} (\bar\zeta_2\cdot\bar\delta_{13})^{\rho_{35}} [\delta\cdot(\bar\zeta_{13} \times \bar\zeta_2)]^{k'_{30}}}{\rho_{32}!\qquad \rho_{33}!\qquad \rho_{35}!\qquad \rho_{36}!\qquad k'_{30}!}, \tag{4.2c}$$

$$h_4 = \Delta_4 \frac{(\zeta_{13}\cdot\bar\zeta_1)^{\rho_{43}} (\zeta_{13}\cdot\bar\zeta_3)^{\rho_{46}} [(\bar\zeta_1 \times \bar\zeta_3)\cdot\delta_{13}]^{k'_{40}}}{\rho_{43}!\qquad \rho_{46}!\qquad k'_{40}!}, \tag{4.2d}$$

where Δ_i is the normalization before the change of variables (the h_i above are not normalized to unity). The degree conditions, Eqs. (3.6), become

$$\begin{aligned} k_{10} &= \mu_{12}, \quad k_{10} + \rho_{11} = \lambda_2, \\ k_{10} + \rho_{12} &= \lambda_1, \quad \rho_{11} + \rho_{12} = \lambda_{12}, \end{aligned} \tag{4.3a}$$

$$k_{20} + \rho_{23} = \mu, \quad k_{20} + \rho_{22} = \lambda_{12}, \quad \rho_{21} + \rho_{22} = \lambda,$$
$$k_{20} + \rho_{21} + \rho_{24} = \lambda_3, \quad \rho_{23} + \rho_{24} = \mu_{12}, \tag{4.3b}$$

$$\rho_{33} + \rho_{36} = \lambda, \quad \rho_{32} + k'_{30} = \mu, \quad \rho_{33} + k'_{30} = \lambda_{13},$$
$$\rho_{32} + \rho_{35} = \mu_{13}, \quad \rho_{35} + \rho_{36} + k'_{30} = \lambda_2, \tag{4.3c}$$

$$\begin{aligned} \rho_{43} + \rho_{46} &= \lambda_{13}, \quad k'_{40} = \mu_{13}, \\ \rho_{46} + k'_{40} &= \lambda_3, \quad \rho_{43} + k'_{40} = \lambda_1. \end{aligned} \tag{4.3d}$$

Note that since $\lambda_1 + \lambda_2 = \lambda_{12} + 2\mu_{12}$ and $\lambda_1 + \lambda_3 = \lambda_{13} + 2\mu_{13}$, therefore $\lambda_{12} + 2\mu_{12} + \lambda_3 = 2\mu_{13} + \lambda_{13} + \lambda_2$ and $\rho_{24} = \rho_{35}$.

Divide the invariants h_i, Eqs. (4.2), by the respective normalizations Δ_i,

$$f_i(\rho_{ij}) \equiv h_i(\rho_{ij})\cdot(\Delta_i)^{-1}. \tag{4.4}$$

Multiply the four $f_k(\rho_{ij})$ by $\prod_{ij} \tau_{ij}^{\rho_{ij}}$ and sum over the ρ_{ij}, then the following generating function $S(\tau_{ij})$

is obtained,

$$S(\tau_{ij}) \equiv \sum \frac{[6(\lambda\mu)]}{\Delta_1 \cdots \Delta_4} \prod \tau_{ij}^{\rho_{ij}} = \int \exp\,[\phi(\tau_{ij};\, \zeta,\, \bar{\zeta})]\, d\mu_{27}(\zeta). \tag{4.5}$$

Conceptually, the remaining steps are clear: integrate over the variables ζ_1, ζ_2, ζ_{12}, ζ'_{12}, ζ_3, ζ, ζ', ζ_{13}, ζ'_{13}, expand in terms of the parameters τ_{ij}, and the coefficient of this expansion is the $6(\lambda\mu)$ symbol divided by the normalizations $\Delta_1 \cdots \Delta_4$. This integration is carried out in the Appendix. The result is

$$[6(\lambda\mu)] = 2C' \cdot S(N_{12}N_{13})^{-\frac{1}{2}}, \tag{4.6}$$

where

$$C' = \left\{\frac{(\lambda_2 - \mu_{12})!\,(\lambda_1 - \mu_{12})!\,k_{20}!\,\rho_{21}!\,\rho_{22}!\,\rho_{23}!\,\rho_{32}!\,\rho_{33}!\,\rho_{35}!\,k'_{30}!\,(\lambda_{12}+1)\,(\lambda_{13}+1)\,(\lambda_1 - \lambda_{13})!\,(\lambda_3 - \lambda_{13})!}{(P+1-\mu_{12})!\,(P+1-\mu_{13})!\,(\lambda+\mu+\lambda_{13}+\mu_{13}+1-P)!\,(\lambda+\mu+\lambda_{12}+\mu_{12}+1-P)!}\right\}^{\frac{1}{2}},$$

$$P = \tfrac{1}{3}(\lambda_{12} + 2\mu_{12} + \lambda_3 + 2\lambda + \mu) \tag{4.7a}$$

and S, in terms of one sum, is

$$S = \sum \frac{(-1)^{\rho_{24}+\lambda_{13}+s}(k_{20}+\rho_{21}+\rho_{22}+\rho_{43}+1-s)!}{s!\,(\rho_{12}-s)!\,(\rho_{43}-s)!\,(\rho_{22}-s)!\,[\rho_{11}-(\rho_{22}-s)]!\,(\rho_{32}-s)!\,(k_{10}-\rho_{24}-\rho_{43}-s)!}. \tag{4.7b}$$

The general $6(\lambda\mu)$ coefficient has not been evaluated yet, though de Swart[1] has calculated certain special cases for high-energy physics applications, and Hecht[8,9] has the coefficients required for shell model calculations.

APPENDIX

The method of evaluating Eq. (4.5) is similar to that of $h_k(\rho_i)$ given in Appendix B of (I), but the calculation is more laborious. Equation (4.5) is first integrated with respect to ζ_{12}, ζ_{13}, ζ'_{12}, ζ'_{13},

$$S(\tau_{ij}) = \int \frac{\exp\,[f(\zeta,\, \tau_{ij})]\, du_{27}}{g(\zeta,\, \tau_{ij})}, \tag{A1}$$

where $g(\zeta, \tau_{ij})$, $f(\zeta, \tau_{ij})$ are functions of the five vectors ζ_1, ζ_2, ζ_3, ζ, ζ', their complex conjugates, and τ_{ij}. The exponential and the denominator may be expanded

$$S(\tau_{ij}) = \sum_{m_i} c(m_i) I_1(m_i,\, \tau_{ij}), \tag{A2}$$

where $c(m_i)$ are the coefficients of the expansion, and $I_1(m_i, \tau_{ij})$ is an integral over a polynomial function of the above vectors. To calculate $I_1(m_i, \tau_{ij})$, multiply it by a set of parameters $\prod (k_i)^{m_i}/m_i!)$ and sum over m_i so that the integrand may again be put in exponential form:

$$S_1(\tau_{ij}) = \sum_{m_i} \prod \left(\frac{(k_i)^{m_i}}{m_i!}\right) I_1(m_i,\, \tau_{ij}) = \int \exp\,[h(\zeta,\, \tau_{ij};\, k_i)]\, d\mu_{15}. \tag{A3}$$

This integral may again be evaluated, expanded, and the above process repeated until all integrations have been performed. Finally, reinserting the results into Eq. (A2), the coefficient of the τ_{ij}'s and the k_i's yield the result, Eq. (4.6).

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Surface-Energy Tensors*

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In this paper the surface-energy tensors are defined and general expressions for their first variations are obtained. These quantities are appropriate for an investigation of the equilibrium and the stability of a charged liquid drop (held together by a constant surface tension) using the method of the tensor virial, which was developed by Chandrasekhar and Lebovitz for the theory of self-gravitating masses. The definitions are shown to be consistent with the conservation laws.

I. INTRODUCTION

THE equilibrium and stability of a rotating, liquid drop held together by surface tension has recently been investigated by Chandrasekhar[1] using an extension of the method of the tensor virial which has found application to a wide variety of problems in the theory of homogeneous masses in gravitational equilibrium. (A summary of these investigations has been given by Chandrasekhar.[2]) In this and in subsequent papers we extend the methods of Ref. 1 along the lines of Ref. 2 to phenomena related to nuclear fission by way of the classical, liquid-drop model of the nucleus.

The theory of stability based on the virial equations presupposes a knowledge of various tensor quantities related to the surface energy and the electrostatic potential-energy. The purpose of this paper is to assemble in one place in a common, systematic notation, the necessary formulas related to the surface energy which are appropriate for an investigation of stability using the virial method. Owing to the formal similarity between gravitation and electrostatics, the necessary formulas related to the electrostatic potential-energy can readily be obtained from the formalism previously developed in the context of gravitation by Chandrasekhar and Lebovitz.[3,4] The notation used in the two theories is compared in the Appendix.

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II. SURFACE-ENERGY TENSORS; VIRIAL THEOREMS

We first briefly review the steps described in Ref. 1 which lead to the natural appearance of the surface-energy tensor in the virial theorem of the second order.

Consider a uniformly charged fluid confined to a volume V bounded by a *closed* surface $\mathbf{S}$ on which surface tension (of constant magnitude T) is operative. Assume that the external pressure on $\mathbf{S}$ is zero. The pressure in the interior, immediately adjacent to $\mathbf{S}$, is given by Laplace's formula

$$p = T \operatorname{div} \mathbf{n} \qquad (\text{on } \mathbf{S}), \tag{1}$$

where $\mathbf{n}$ is the unit outward normal on $\mathbf{S}$. Interior to $\mathbf{S}$ and in the volume V, the equation of motion governing the fluid having mass density ρ and positive charge density σ is

$$\rho\, du_i/dt = -\partial p/\partial x_i - \sigma\, \partial \mathfrak{V}/\partial x_i, \tag{2}$$

where u_i denotes the velocity and $\mathfrak{V}$ is the electrostatic potential defined in the Appendix.

The virial theorem of the second order is obtained by first multiplying Eq. (2) by x_j and then integrating the result over the volume V. By transformations described in Ref. 2, one obtains

$$\frac{d}{dt}\int_V \rho u_i x_j\, d\tau = 2\mathfrak{T}_{ij} - \int_V x_j \frac{\partial p}{\partial x_i}\, d\tau + \mathfrak{W}_{ij}\,, \tag{3}$$

where

$$\mathfrak{T}_{ij} = \frac{1}{2}\int_V \rho u_i u_j\, d\tau \tag{4}$$

is the kinetic-energy tensor and $\mathfrak{W}_{ij}$ is the electrostatic potential-energy tensor defined in the Appendix. One can integrate by parts the term in Eq. (3) which contains the pressure gradient, and use Eq. (1) to obtain

$$-\int_V x_j \frac{\partial p}{\partial x_i}\, d\tau = -T\int_S x_j \operatorname{div} \mathbf{n}\, dS_i + \Pi\, \delta_{ij}, \tag{5}$$

where

$$\Pi = \int_V p \, d\tau \tag{6}$$

and

$$dS_i = n_i \, dS \tag{7}$$

is the vector element of area on S.

We define the surface-energy tensor $\mathfrak{S}_{ij}$ by

$$\mathfrak{S}_{ij} \equiv \tfrac{1}{2}T \int_S x_j \operatorname{div} \mathbf{n} \, dS_i. \tag{8}$$

(This differs by a factor of $-\frac{1}{2}$ from the corresponding definition chosen by Chandrasekhar in Ref. 1.)

In Ref. 1 the surface-energy tensor was shown to be symmetric in i and j, as required by the conservation of angular momentum. An alternative demonstration of this symmetry is possible which, moreover, leads to a simpler form of $\mathfrak{S}_{ij}$ that is more suitable for purposes of explicit evaluation. The following lemma is useful for this purpose.

Lemma: Let **F** be an arbitrary vector defined on a closed surface S. Then

$$\int_S \frac{\partial F_l}{\partial x_l} \, dS_i = \int_S \frac{\partial F_l}{\partial x_i} \, dS_l. \tag{9}$$

(The summation convention applies to repeated indices.)

Proof: By Stokes's theorem on a closed surface

$$\epsilon_{kmn} \int_S \frac{\partial A_n}{\partial x_m} \, dS_k = 0 \qquad \text{(closed surface)}. \tag{10}$$

Since **A** is arbitrary, choose it to have the form

$$A_n = \epsilon_{nil} F_l. \tag{11}$$

(The presence of the extra index i is immaterial in this context.) Then

$$\begin{aligned} 0 &= \epsilon_{kmn}\epsilon_{nil} \int_S \frac{\partial F_l}{\partial x_m} \, dS_k \\ &= (\delta_{ki}\,\delta_{ml} - \delta_{kl}\,\delta_{mi}) \int_S \frac{\partial F_l}{\partial x_m} \, dS_k \\ &= \int_S \frac{\partial F_l}{\partial x_l} \, dS_i - \int_S \frac{\partial F_l}{\partial x_i} \, dS_l \, , \end{aligned} \tag{12}$$

which establishes the lemma.

Now choose[5]

$$F_l = n_l x_j, \tag{13}$$

and apply the lemma to obtain

$$\begin{aligned} \int_S x_j \operatorname{div} \mathbf{n} \, dS_i &= \int_S x_j \frac{\partial n_l}{\partial x_i} n_l \, dS \\ &\quad + \delta_{ij} \int_S n_l \, dS_l - \int_S n_j \, dS_i \\ &= \delta_{ij} \int_S dS - \int_S n_i n_i \, dS. \end{aligned} \tag{14}$$

In view of Eq. (8), we obtain

$$\mathfrak{S}_{ij} = \tfrac{1}{2}T \int_S (\delta_{ij} - n_i n_j) \, dS. \tag{15}$$

This expression is manifestly symmetric in i and j. Moreover, the trace of $\mathfrak{S}_{ij}$ is

$$\mathfrak{S}_{ii} \equiv \mathfrak{S} = T \int_S dS = T\mathfrak{a}, \tag{16}$$

where $\mathfrak{a}$ is the total area of the surface S. The quantity $\mathfrak{S}$ agrees with the usual thermodynamic definition of the surface energy.

The virial theorem of the second order for a nonrotating charged liquid drop thus takes the form[6]

$$\frac{d}{dt} \int_V \rho u_i x_j \, d\tau = 2\mathfrak{T}_{ij} - 2\mathfrak{S}_{ij} + \mathfrak{W}_{ij} + \Pi \, \delta_{ij}. \tag{17}$$

The virial theorem of the third order is obtained by first multiplying Eq. (2) by $x_j x_k$ and then integrating the result over the volume V. The following discussion is confined to the term which contains the pressure gradient. (For a discussion of the other terms in the resulting virial equation, see Ref. 2, Chap. 2.) This term can be written in the form

$$\begin{aligned} -\int_V x_j x_k \frac{\partial p}{\partial x_i} \, d\tau &= -T \int_S x_j x_k \operatorname{div} \mathbf{n} \, dS_i \\ &\quad + \delta_{ij} \Pi_k + \delta_{ik} \Pi_j, \end{aligned} \tag{18}$$

where

$$\Pi_i = \int_V x_i p \, d\tau. \tag{19}$$

If we now choose

$$F_l = n_l x_j x_k, \tag{20}$$

then the lemma can be used to transform the surface integral in Eq. (18) into the form

$$-T \int_S x_j x_k \operatorname{div} \mathbf{n} \, dS_i = -2\mathfrak{S}_{ij;k} - 2\mathfrak{S}_{ik;j}, \tag{21}$$

where we have defined the surface-energy tensor appropriate to the third order as

$$\mathfrak{S}_{ij;k} \equiv \tfrac{1}{2}T \int_S (\delta_{ij} - n_i n_j) x_k \, dS. \tag{22}$$

[5] Again the presence of the extra index j does not affect the application of the lemma.

[6] See Ref. 1, Eq. (10).

This tensor is manifestly symmetric in i and j. (The index following the semicolon indicates that a moment with respect to the associated space coordinate is involved.) It is the appropriate analog of the other tensor quantities of the third order, such as $\mathfrak{T}_{ij;k}$ and $\mathfrak{W}_{ij;k}$, which are defined in Ref. 2. [See also Eq. (A6) in the Appendix.]

The virial theorem of the third order for a nonrotating charged liquid drop takes the form[7]

$$\frac{d}{dt}\int_V \rho u_i x_j x_k \, d\tau = 2(\mathfrak{T}_{ij;k} + \mathfrak{T}_{ik;j}) - 2(\mathfrak{S}_{ij;k} + \mathfrak{S}_{ik;j}) + \mathfrak{W}_{ij;k} + \mathfrak{W}_{ik;j} + \delta_{ij}\,\Pi_k + \delta_{ik}\,\Pi_j. \tag{23}$$

The extension of Eqs. (17) and (23) to include rotation is given in Ref. 2.

III. FIRST VARIATIONS OF $\mathfrak{S}_{ij}$ AND $\mathfrak{S}_{ij;k}$

Suppose that the liquid drop, initially in a state of equilibrium, is slightly perturbed; and further that the ensuing motions are described by a Lagrangian displacement $\xi(\mathbf{x}, t)$. The first variations of the surface-energy tensors $\delta\mathfrak{S}_{ij}$ and $\delta\mathfrak{S}_{ij;k}$ due to the deformations caused by the displacement ξ, are needed for an investigation of stability.

By definition,

$$\delta\mathfrak{S}_{ij} \equiv \tfrac{1}{2}T\delta\int_S (\delta_{ij} - n_i n_j)\, dS. \tag{24}$$

Since the operations of displacement and integration commute, the relation

$$\delta[(\delta_{ij} - n_i n_j)\, dS] = \delta_{ij}\,\delta(dS) - \delta n_j\, dS_i - n_j\,\delta(dS_i) \tag{25}$$

can be used to express Eq. (24) in the form

$$\delta\mathfrak{S}_{ij} = \tfrac{1}{2}T\Big[\delta_{ij}\int_S \delta(dS) - \int_S \delta n_j\, dS_i - \int_S n_j\,\delta(dS_i)\Big]. \tag{26}$$

The expression for $\delta(dS_i)$ in terms of ξ,

$$\delta(dS_i) = \operatorname{div}\xi\, dS_i - (\partial\xi_l/\partial x_i)\, dS_l, \tag{27}$$

was derived in Ref. 1. By substituting Eq. (27) into

$$\delta(dS) = \delta(n_m\, dS_m) = n_m\,\delta(dS_m) + n_m\,\delta n_m\, dS = n_m\,\delta(dS_m), \tag{28}$$

one obtains

$$\delta(dS) = \{\operatorname{div}\xi - [n_l n_m(\partial\xi_l/\partial x_m)]\}\, dS. \tag{29}$$

[7] See Ref. 2, Chap. 2, Eq. (15).

By substituting Eqs. (27) and (29) into

$$\delta n_i\, dS = \delta(dS_i) - n_i\,\delta(dS), \tag{30}$$

one obtains

$$\delta n_i = \{n_i[n_l n_m(\partial\xi_l/\partial x_m)] - n_l(\partial\xi_l/\partial x_i)\}. \tag{31}$$

The substitution of Eqs. (27), (29), and (31) into Eq. (26) yields the desired result:

$$\delta\mathfrak{S}_{ij} = -\tfrac{1}{2}T\int_S (\delta_{ij} + n_i n_j)\Big(n_l n_m \frac{\partial\xi_l}{\partial x_m}\Big)\, dS + \tfrac{1}{2}T\int_S \Big(n_i\frac{\partial\xi_l}{\partial x_j} + n_j\frac{\partial\xi_l}{\partial x_i}\Big)n_l\, dS + \tfrac{1}{2}T\int_S (\delta_{ij} - n_i n_j)\operatorname{div}\xi\, dS. \tag{32}$$

By definition,

$$\delta\mathfrak{S}_{ij;k} \equiv \tfrac{1}{2}T\,\delta\int_S (\delta_{ij} - n_i n_j)x_k\, dS \tag{33}$$

$$= \tfrac{1}{2}T\int_S (\delta_{ij} - n_i n_j)\xi_k\, dS + \tfrac{1}{2}T\int_S x_k\,\delta[(\delta_{ij} - n_i n_j)\, dS]. \tag{34}$$

The last term in Eq. (34) can be evaluated by using Eqs. (25), (27), (29), and (31). The result is

$$\delta\mathfrak{S}_{ij;k} = \tfrac{1}{2}T\int_S (\delta_{ij} - n_i n_j)\xi_k\, dS - \tfrac{1}{2}T\int_S (\delta_{ij} + n_i n_j)\Big(n_l n_m\frac{\partial\xi_l}{\partial x_m}\Big)x_k\, dS + \tfrac{1}{2}T\int_S \Big(n_i\frac{\partial\xi_l}{\partial x_j} + n_j\frac{\partial\xi_l}{\partial x_i}\Big)n_l x_k\, dS + \tfrac{1}{2}T\int_S (\delta_{ij} - n_i n_j)x_k\operatorname{div}\xi\, dS. \tag{35}$$

The last term in each of Eqs. (32) and (35), which contains div ξ, vanishes if the fluid is incompressible.

Equations (32) and (35) can be written alternatively in the form

$$\delta\mathfrak{S}_{ij} = \tfrac{1}{2}T\int_S (\xi\cdot\mathbf{n})\Big[\delta_{ij}\frac{\partial n_m}{\partial x_m} + \frac{\partial}{\partial x_m}(n_m n_i n_j) - \frac{\partial n_i}{\partial x_j} - \frac{\partial n_j}{\partial x_i}\Big]\, dS \tag{36}$$

and

$$\delta\mathfrak{S}_{ij;k} = \tfrac{1}{2}T\int_S (\xi\cdot\mathbf{n})\Big[\delta_{ij}\frac{\partial}{\partial x_m}(n_m x_k) + \frac{\partial}{\partial x_m}(n_m n_i n_j x_k) - \frac{\partial}{\partial x_j}(n_i x_k) - \frac{\partial}{\partial x_i}(n_j x_k)\Big]\, dS, \tag{37}$$

which, formally, does not distinguish between the compressible and incompressible cases.

IV. CONSERVATION LAWS

It is of some interest to show that the concept of the surface-energy tensor, as formulated in Sec. II, is consistent with the well-known conservation laws of linear momentum, of angular momentum, and of energy. In what follows we confine our attention to the terms arising from the inclusion of the pressure gradient in the equation of motion, and refer the reader to Ref. 2 for a discussion of all the other terms.

The conservation of angular momentum follows immediately from the tensor form of the virial theorem of the second order, given by Eq. (17), as a direct consequence of the symmetry of the right-hand side of this equation.

The conservation of linear momentum is obtained by directly integrating the equation of motion over the volume occupied by the fluid. The integral over the pressure gradient vanishes when use is made of Eq. (1) and the lemma:

$$\int_V \frac{\partial p}{\partial x_i}\, d\tau = \int_S p\, dS_i$$

$$= T \int_S \frac{\partial n_l}{\partial x_l}\, dS_i = T \int_S \frac{\partial n_l}{\partial x_i}\, n_l\, dS = 0. \qquad (38)$$

The energy integral is obtained by first multiplying the equation of motion by u_i, then summing over i, and finally integrating over V. The term arising from the pressure gradient can be integrated by parts to obtain

$$-\int_V u_i \frac{\partial p}{\partial x_i}\, d\tau$$

$$= -\int_S u_i p\, dS_i + \int_S p\, \mathrm{div}\, \mathbf{u}\, d\tau. \qquad (39)$$

The term in Eq. (39) which contains div $\mathbf{u}$ vanishes if the fluid is incompressible. Otherwise, it is related to the time rate of change of the internal energy. For example, if the pressure and density of the fluid are related by an adiabatic equation of state, then one has

$$\int_V p\, \mathrm{div}\, \mathbf{u}\, d\tau = -\frac{1}{\gamma - 1}\frac{d\Pi}{dt}, \qquad (40)$$

where γ is the constant ratio of specific heats and Π is given by Eq. (6).

The surface integral in Eq. (39) can be transformed as follows:

$$-\int_S u_i p\, dS_i = -T \int_S u_i \frac{\partial n_l}{\partial x_l}\, dS_i$$

$$= -T \int_S \frac{\partial}{\partial x_l}(u_i n_l)\, dS_i + T \int \left(n_i n_l \frac{\partial u_i}{\partial x_l}\right) dS$$

$$= -T \int_S \frac{\partial}{\partial x_i}(u_i n_l)\, dS_l + T \int_S \left(n_i n_l \frac{\partial u_i}{\partial x_l}\right) dS$$

(by using the lemma)

$$= -T \int_S \left[\frac{\partial u_l}{\partial x_i} - \left(n_i n_l \frac{\partial u_i}{\partial x_l}\right)\right] dS \qquad (41)$$

$$= -T \int_S \frac{d}{dt}(dS) = -\frac{d}{dt}(T\mathfrak{A}), \qquad (42)$$

where the first expression in Eq. (42) is obtained by comparing Eq. (41) with Eq. (28). This confirms that $\mathfrak{S}$, defined by Eq. (16), is indeed the surface energy.

The complete energy integral for a nonrotating incompressible charged liquid drop follows from

$$(d/dt)(\mathfrak{T} + \mathfrak{W} + \mathfrak{S}) = 0, \qquad (43)$$

where $\mathfrak{T}$ is the kinetic energy given by the trace of Eq. (4) and $\mathfrak{W}$ is the electrostatic potential-energy given by the trace of $\mathfrak{W}_{ij}$ defined in the Appendix. The generalization of this result to include rotation is straightforward.

V. CONCLUDING REMARKS

In this paper we defined the surface-energy tensors and obtained general expressions for their first variations which are appropriate for investigation of the stability of a charged liquid drop by using the tensor form of the virial equations. In a subsequent paper we shall evaluate these expressions for the particular case that the equilibrium shape is *assumed* to be a tri-axial ellipsoid.

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APPENDIX. POTENTIAL-ENERGY TENSORS

In view of the formal similarity between gravitation and electrostatics, the electrostatic potential and all of the quantities related to it can be evaluated by using the formalism previously developed by Chandrasekhar and Lebovitz[2-4] for potentials and superpotentials in the theory of gravitation. In order to obtain the desired formulas appropriate for a charged fluid with charge density $\sigma(\mathbf{x})$ from the formulas in Refs. 2–4 for a self-gravitating

fluid with mass density $\rho(\mathbf{x})$, only the signs of the force, of the potential energy, and of the various potential-energy tensors need to be changed. The signs of the potential, of the tensor potentials, and of the superpotentials remain unchanged.

The following list serves to define the quantities needed in this and in subsequent papers. The electrostatic force per unit volume is

$$-\sigma\,\partial\mathfrak{V}/\partial x_i, \tag{A1}$$

where

$$\mathfrak{V}(\mathbf{x}) = \int_V \frac{\sigma(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\,d\tau' \tag{A2}$$

is the potential. The tensor potential is

$$\mathfrak{V}_{ij}(\mathbf{x}) = \int_V \sigma(x')\,\frac{(x_i-x_i')(x_j-x_j')}{|\mathbf{x}-\mathbf{x}'|^3}\,d\tau'. \tag{A3}$$

The potential energy is

$$\mathfrak{W} = -\int_V \sigma x_i\,\frac{\partial\mathfrak{V}}{\partial x_i}\,d\tau = \frac{1}{2}\int_V \sigma\mathfrak{V}\,d\tau, \tag{A4}$$

the potential-energy tensor of the second order is

$$\mathfrak{W}_{ij} = -\int_V \sigma x_j\,\frac{\partial\mathfrak{V}}{\partial x_i}\,d\tau = \frac{1}{2}\int_V \sigma\mathfrak{V}_{ij}\,d\tau, \tag{A5}$$

and the potential-energy tensor of the third order is

$$\mathfrak{W}_{ij;k} = \frac{1}{2}\int_V \sigma\mathfrak{V}_{ij}x_k\,d\tau. \tag{A6}$$

(The index following the semicolon in $\mathfrak{W}_{ij;k}$ indicates that a moment with respect to the associated space coordinate is involved.)

The first variations $\delta\mathfrak{W}_{ij}$ and $\delta\mathfrak{W}_{ij;k}$ due to an infinitesimal deformation of a configuration by a Lagrangian displacement ξ are given by

$$\delta\mathfrak{W}_{ij} = \int_V \sigma\xi_l\,\frac{\partial\mathfrak{V}_{ij}}{\partial x_l}\,d\tau \tag{A7}$$

and

$$2\delta\mathfrak{W}_{ij;k} = \int_V \sigma\xi_k\mathfrak{V}_{ij}\,d\tau + \int_V \sigma x_k\xi_l\,\frac{\partial\mathfrak{V}_{ij}}{\partial x_l}\,d\tau + \int_V \sigma\xi_l\,\frac{\partial\mathfrak{D}_{ij;k}}{\partial x_l}\,d\tau, \tag{A8}$$

where $\mathfrak{D}_{ij;k}$ is the tensor

$$\mathfrak{D}_{ij;k} = \int_V \sigma(\mathbf{x}')\,\frac{(x_i-x_i')(x_j-x_j')x_k'}{|\mathbf{x}-\mathbf{x}'|^3}\,d\tau'. \tag{A9}$$

These formulas are entirely general and not limited to homogeneous configurations.

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Surface-Energy Tensors for Ellipsoids*

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The surface-energy tensors are evaluated for ellipsoidal surfaces in terms of particular types of elliptic integrals which have simple algebraic recursion relations that are useful for numerical evaluation. The final expressions are given in a form appropriate for an investigation of stability using the method of the tensor virial.

I. INTRODUCTION

GENERAL expressions for the surface-energy tensors were derived in a previous paper.[1] These quantities are appropriate for an investigation of the equilibrium and the stability of a charged liquid drop (held together by a constant surface tension) using the method of the tensor virial, which was developed by Chandrasekhar and Lebovitz for the theory of self-gravitating masses.[2] In this paper we evaluate the surface-energy tensors for ellipsoidal surfaces. (The relevance of this particular surface to our subsequent investigations of stability is outlined in Appendix D.)

All of the surface-energy tensors for ellipsoids

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[2] For a summary of these investigations see S. Chandrasekhar, in *Lectures in Theoretical Physics*, W. E. Brittin and W. R. Chappell, Eds. (University of Colorado Press, Boulder, Colorado, 1964), Vol. 6, p. 1.

fluid with mass density $\rho(\mathbf{x})$, only the signs of the force, of the potential energy, and of the various potential-energy tensors need to be changed. The signs of the potential, of the tensor potentials, and of the superpotentials remain unchanged.

The following list serves to define the quantities needed in this and in subsequent papers. The electrostatic force per unit volume is

$$-\sigma\,\partial\mathfrak{V}/\partial x_i, \tag{A1}$$

where

$$\mathfrak{V}(\mathbf{x}) = \int_V \frac{\sigma(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\,d\tau' \tag{A2}$$

is the potential. The tensor potential is

$$\mathfrak{V}_{ij}(\mathbf{x}) = \int_V \sigma(x')\,\frac{(x_i-x_i')(x_j-x_j')}{|\mathbf{x}-\mathbf{x}'|^3}\,d\tau'. \tag{A3}$$

The potential energy is

$$\mathfrak{W} = -\int_V \sigma x_i\,\frac{\partial\mathfrak{V}}{\partial x_i}\,d\tau = \frac{1}{2}\int_V \sigma\mathfrak{V}\,d\tau, \tag{A4}$$

the potential-energy tensor of the second order is

$$\mathfrak{W}_{ij} = -\int_V \sigma x_j\,\frac{\partial\mathfrak{V}}{\partial x_i}\,d\tau = \frac{1}{2}\int_V \sigma\mathfrak{V}_{ij}\,d\tau, \tag{A5}$$

and the potential-energy tensor of the third order is

$$\mathfrak{W}_{ij;k} = \frac{1}{2}\int_V \sigma\mathfrak{V}_{ij}x_k\,d\tau. \tag{A6}$$

(The index following the semicolon in $\mathfrak{W}_{ij;k}$ indicates that a moment with respect to the associated space coordinate is involved.)

The first variations $\delta\mathfrak{W}_{ij}$ and $\delta\mathfrak{W}_{ij;k}$ due to an infinitesimal deformation of a configuration by a Lagrangian displacement ξ are given by

$$\delta\mathfrak{W}_{ij} = \int_V \sigma\xi_l\,\frac{\partial\mathfrak{V}_{ij}}{\partial x_l}\,d\tau \tag{A7}$$

and

$$2\delta\mathfrak{W}_{ij;k} = \int_V \sigma\xi_k\mathfrak{V}_{ij}\,d\tau + \int_V \sigma x_k\xi_l\,\frac{\partial\mathfrak{V}_{ij}}{\partial x_l}\,d\tau + \int_V \sigma\xi_l\,\frac{\partial\mathfrak{D}_{ij;k}}{\partial x_l}\,d\tau, \tag{A8}$$

where $\mathfrak{D}_{ij;k}$ is the tensor

$$\mathfrak{D}_{ij;k} = \int_V \sigma(\mathbf{x}')\,\frac{(x_i-x_i')(x_j-x_j')x_k'}{|\mathbf{x}-\mathbf{x}'|^3}\,d\tau'. \tag{A9}$$

These formulas are entirely general and not limited to homogeneous configurations.

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Surface-Energy Tensors for Ellipsoids*

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The surface-energy tensors are evaluated for ellipsoidal surfaces in terms of particular types of elliptic integrals which have simple algebraic recursion relations that are useful for numerical evaluation. The final expressions are given in a form appropriate for an investigation of stability using the method of the tensor virial.

I. INTRODUCTION

GENERAL expressions for the surface-energy tensors were derived in a previous paper.[1] These quantities are appropriate for an investigation of the equilibrium and the stability of a charged liquid drop (held together by a constant surface tension) using the method of the tensor virial, which was developed by Chandrasekhar and Lebovitz for the theory of self-gravitating masses.[2] In this paper we evaluate the surface-energy tensors for ellipsoidal surfaces. (The relevance of this particular surface to our subsequent investigations of stability is outlined in Appendix D.)

All of the surface-energy tensors for ellipsoids

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[1] C. E. Rosenkilde, J. Math. Phys. 8, 84 (1967).

[2] For a summary of these investigations see S. Chandrasekhar, in *Lectures in Theoretical Physics*, W. E. Brittin and W. R. Chappell, Eds. (University of Colorado Press, Boulder, Colorado, 1964), Vol. 6, p. 1.

can be evaluated in terms of particular types of elliptic integrals which are designated by multi-index symbols. These symbols satisfy algebraic recursion relations that closely resemble the relations satisfied by the "multi-index symbols" which were developed by Chandrasekhar and Lebovitz[3] for evaluating the potentials and superpotentials of homogeneous ellipsoids in the theory of gravitation. The two types of multi-index symbols are compared in Appendix B. The principal advantage in using these symbols is their computational utility; a knowledge of only the three one-index symbols is sufficient for the numerical evaluation of all higher-order symbols via the algebraic recursion relations derived in Sec. II.

The transformation introduced in Sec. III simplifies the angular integration in all of the subsequent integrals. By using this transformation we may express all the formulas, which were derived in Ref. 1, in terms of the multi-index symbols. The final expressions obtained for the surface-energy tensors are in a form that is appropriate for an investigation of the stability of an incompressible liquid drop that is initially homogeneous. The additional terms that are needed if the fluid is compressible are evaluated in Appendix C.

It is important to state here at the outset that in this paper the summation convention over repeated indices is *not adopted*: summation, whenever required, is indicated explicitly. In all cases the limits on the summations, which run from 1 to 3, are omitted.

II. MULTI-INDEX SYMBOLS

Consider an ellipsoid with semiaxes a_1, a_2, and a_3; and suppose, in the first instance, that the a_i's are all different. The case when $a_1 = a_2$ (say) is degenerate and is treated separately.

We define the integrals

$$\mathcal{I} \equiv \int_0^\infty \frac{dt}{\Delta}, \tag{1}$$

$$\mathfrak{A}_{ijk\cdots} \equiv \int_0^\infty \frac{dt}{\Delta(a_i^2+t^2)(a_j^2+t^2)(a_k^2+t^2)\cdots}, \tag{2}$$

and

$$\mathfrak{B}_{ijk\cdots} \equiv \int_0^\infty \frac{t^2\,dt}{\Delta(a_i^2+t^2)(a_j^2+t^2)(a_k^2+t^2)\cdots}, \tag{3}$$

where

$$\Delta^2 = (a_1^2+t^2)(a_2^2+t^2)(a_3^2+t^2). \tag{4}$$

[3] S. Chandrasekhar and N. R. Lebovitz, Astrophys. J. **136**, 1037 (1962).

As defined, $\mathfrak{A}_{ijk\cdots}$ and $\mathfrak{B}_{ijk\cdots}$ are completely symmetric in their indices. The indices may assume any of the values 1 to 3. We are mostly interested in the symbols with three or fewer indices.

A. One-Index Symbols $\mathfrak{A}_i$ and $\mathfrak{B}_i$

By definition,

$$\mathfrak{A}_i \equiv \int_0^\infty \frac{dt}{\Delta(a_i^2+t^2)} \text{ and } \mathfrak{B}_i \equiv \int_0^\infty \frac{t^2\,dt}{\Delta(a_i^2+t^2)}. \tag{5}$$

Clearly,

$$\mathfrak{B}_i = \int_0^\infty \frac{[(a_i^2+t^2)-a_i^2]\,dt}{\Delta(a_i^2+t^2)} = \mathcal{I} - a_i^2\mathfrak{A}_i. \tag{6}$$

We verify that

$$\frac{\partial \mathcal{I}}{\partial a_i^2} = -\frac{1}{2}\int_0^\infty \frac{dt}{\Delta(a_i^2+t^2)} = -\tfrac{1}{2}\mathfrak{A}_i \qquad (a_1 \neq a_2 \neq a_3). \tag{7}$$

Since $\mathcal{I}$ is a homogeneous function of degree -1 in a_i^2, we have, by Euler's theorem,

$$\sum_i a_i^2 \frac{\partial \mathcal{I}}{\partial a_i^2} = -\mathcal{I}, \tag{8}$$

or in view of Eq. (7),

$$\sum_i a_i^2\mathfrak{A}_i = 2\mathcal{I}. \tag{9}$$

By using Eqs. (6) and (9), we obtain

$$\sum_i \mathfrak{B}_i = 3\mathcal{I} - \sum_i a_i^2\mathfrak{A}_i = \mathcal{I}, \tag{10}$$

$$\mathfrak{B}_i + \mathfrak{B}_j = 2\mathcal{I} - (a_i^2\mathfrak{A}_i + a_j^2\mathfrak{A}_j) = a_k^2\mathfrak{A}_k, \tag{11}$$

and

$$2\mathfrak{B}_i = 2\mathcal{I} - 2a_i^2\mathfrak{A}_i = a_j^2\mathfrak{A}_j + a_k^2\mathfrak{A}_k - a_i^2\mathfrak{A}_i. \tag{12}$$

Equations (11), (12), and all subsequent identities in which the indices i, j, and k appear together, are understood to apply in their most *general* form to ellipsoids with $a_1 \neq a_2 \neq a_3$; the indices i, j, and k may take any of the values 1, 2, or 3, but with $i \neq j \neq k$. However, from the definitions of the multi-index symbols, it is clear that for spheroids, either oblate ($a_1 = a_2 > a_3$, say) or prolate ($a_1 = a_2 < a_3$, say), no ambiguity results if every "2" is replaced by a "1" wherever it appears. (Thus, $\mathfrak{A}_1 = \mathfrak{A}_2 \neq \mathfrak{A}_3$ and $\mathfrak{B}_1 = \mathfrak{B}_2 \neq \mathfrak{B}_3$ for this particular case.) Moreover, each of the identities (unless otherwise noted) applies equally well to the more restricted case of spheroids. Thus, Eqs. (11) and (12) become identical when $i = j$.

Equation (12) shows that all the $\mathfrak{B}_i$'s can be evaluated numerically, once the three $\mathfrak{A}_i$'s are known.

The three $\mathfrak{A}_i$'s can be evaluated in terms of incomplete elliptic integrals of the first and second kinds as shown in Appendix A. When $a_1 = a_2$, the integrals become elementary; formulas appropriate for both oblate and prolate spheroids are also given in Appendix A.

B. Two-Index Symbols $\mathfrak{A}_{ij}$ and $\mathfrak{B}_{ij}$

By definition,

$$\mathfrak{A}_{ij} \equiv \int_0^\infty \frac{dt}{\Delta(a_i^2 + t^2)(a_j^2 + t^2)}, \qquad \mathfrak{B}_{ij} \equiv \int_0^\infty \frac{t^2\,dt}{\Delta(a_i^2 + t^2)(a_j^2 + t^2)}. \tag{13}$$

Clearly [cf. Eq. (6)],

$$\mathfrak{B}_{ij} = \mathfrak{A}_i - a_j^2\mathfrak{A}_{ji} = \mathfrak{A}_j - a_i^2\mathfrak{A}_{ij}. \tag{14}$$

Because $\mathfrak{A}_{ij}$ and $\mathfrak{B}_{ij}$ are symmetric in i and j, it follows from Eq. (14) that

$$(a_i^2 - a_j^2)\mathfrak{A}_{ij} = -(\mathfrak{A}_i - \mathfrak{A}_j), \tag{15}$$

$$(a_i^2 - a_j^2)\mathfrak{B}_{ij} = a_i^2\mathfrak{A}_i - a_j^2\mathfrak{A}_j. \tag{16}$$

Equations (15) and (16) determine the two-index symbols with $i \neq j$ in terms of the one-index symbols.

The three two-index symbols with $i \neq j$ are not independent since

$$(a_1^2 - a_2^2)\mathfrak{A}_{12} + (a_2^2 - a_3^2)\mathfrak{A}_{23} + (a_3^2 - a_1^2)\mathfrak{A}_{31} = 0, \tag{17}$$

$$(a_1^2 - a_2^2)\mathfrak{B}_{12} + (a_2^2 - a_3^2)\mathfrak{B}_{23} + (a_3^2 - a_1^2)\mathfrak{B}_{31} = 0. \tag{18}$$

Expressions having exactly this form were obtained by Jellet.[4]

To determine $\mathfrak{A}_{ii}$ and $\mathfrak{B}_{ii}$, we observe that the one-index symbols, $\mathfrak{A}_i$ and $\mathfrak{B}_i$, are homogeneous functions of degree -2 and -1, respectively, in a_i^2; hence by Euler's theorem, we have

$$4\mathfrak{A}_i = 3a_i^2\mathfrak{A}_{ii} + a_j^2\mathfrak{A}_{ji} + a_k^2\mathfrak{A}_{ki}, \tag{19}$$

$$2\mathfrak{B}_i = 3a_i^2\mathfrak{B}_{ii} + a_j^2\mathfrak{B}_{ji} + a_k^2\mathfrak{B}_{ki}. \tag{20}$$

In view of Eq. (14), two alternative forms of Eq. (19) are

$$\mathfrak{A}_i = 3\mathfrak{B}_{ii} + \mathfrak{B}_{ij} + \mathfrak{B}_{ik}, \tag{21}$$

$$2\mathfrak{A}_i + \mathfrak{A}_j + \mathfrak{A}_k = a_i^2(3\mathfrak{A}_{ii} + \mathfrak{A}_{ij} + \mathfrak{A}_{ik}). \tag{22}$$

[4] J. H. Jellet, Cambridge and Dublin Math. J. 1, 57 (1846). His symbols, A_i, are areas of particular portions of the surface of an ellipsoid and are not the same as our multi-index symbols.

Equations (14), (15), (19), and (21) together determine all the two-index symbols in terms of one-index symbols.

For spheroids ($a_1 = a_2$) it is clear that $\mathfrak{A}_{11} = \mathfrak{A}_{12} = \mathfrak{A}_{22}$, $\mathfrak{A}_{13} = \mathfrak{A}_{23}$, $\mathfrak{B}_{13} = \mathfrak{B}_{23}$, and $\mathfrak{B}_{11} = \mathfrak{B}_{12} = \mathfrak{B}_{22}$.

C. The Three-Index Symbols $\mathfrak{A}_{ijk}$ and $\mathfrak{B}_{ijk}$

Multi-index symbols with any number of indices can be defined and evaluated by using the foregoing techniques. In particular, we need the three-index symbols. Some of the important identities are

$$\mathfrak{B}_{ijk} = \mathfrak{A}_{jk} - a_i^2\mathfrak{A}_{ijk} = \mathfrak{A}_{ik} - a_j^2\mathfrak{A}_{jki} = \mathfrak{A}_{ij} - a_k^2\mathfrak{A}_{kij}, \tag{23}$$

$$(a_i^2 - a_j^2)\mathfrak{A}_{ijk} = -(\mathfrak{A}_{ik} - \mathfrak{A}_{jk}), \tag{24}$$

$$(a_i^2 - a_k^2)\mathfrak{A}_{ikk} = -(\mathfrak{A}_{ik} - \mathfrak{A}_{kk}), \tag{25}$$

$$6\mathfrak{A}_{ii} = 5a_i^2\mathfrak{A}_{iii} + a_j^2\mathfrak{A}_{jii} + a_k^2\mathfrak{A}_{kii}, \tag{26}$$

$$6\mathfrak{A}_{ij} = 3(a_i^2\mathfrak{A}_{iij} + a_j^2\mathfrak{A}_{jij}) + a_k^2\mathfrak{A}_{kij}, \tag{27}$$

$$\mathfrak{A}_{ii} = 5\mathfrak{B}_{iii} + \mathfrak{B}_{jii} + \mathfrak{B}_{kii}, \tag{28}$$

$$\mathfrak{A}_{ij} = 3(\mathfrak{B}_{iij} + \mathfrak{B}_{jij}) + \mathfrak{B}_{kij}, \tag{29}$$

$$4\mathfrak{A}_{ii} + \mathfrak{A}_{ij} + \mathfrak{A}_{ik} = a_i^2(5\mathfrak{A}_{iii} + \mathfrak{A}_{iij} + \mathfrak{A}_{iik}). \tag{30}$$

The identities obtained in Sec. II are sufficient for the numerical evaluation of all the multi-index symbols with two or three indices given the values of the three one-index symbols, $\mathfrak{A}_1$, $\mathfrak{A}_2$, and $\mathfrak{A}_3$. These identities are also useful in transforming and simplifying the expressions which we obtain for the surface-energy tensors.

III. A TRANSFORMATION

The unit outward normal of the ellipsoidal surface

$$\frac{x_1^2}{a_1^2} + \frac{x_2^2}{a_2^2} + \frac{x_3^2}{a_3^2} - 1 = 0 \tag{31}$$

has components

$$n_i = x_i p/a_i^2, \tag{32}$$

where

$$p = \left(\frac{x_1^2}{a_1^4} + \frac{x_2^2}{a_2^4} + \frac{x_3^2}{a_3^4}\right)^{-\frac{1}{2}}. \tag{33}$$

The element of area dS, in terms of its projected area on each of the coordinate planes, is

$$dS = dx_i\,dx_j/|n_k| \qquad (i \neq j \neq k). \tag{34}$$

[In order to avoid any ambiguities in the use of Eq. (34) due to the sign of n_k, we restrict our attention to the positive hemisphere (S^+) involved

and take advantage of the triplanar symmetry of the ellipsoid.] Since the three expressions (34) are equivalent, choose $i = 1$, $j = 2$, and $k = 3$, and introduce the transformation

$$x_1 = a_1^2(a_1^2 + t^2)^{-\frac{1}{2}} \cos\varphi, \qquad x_2 = a_2^2(a_2^2 + t^2)^{-\frac{1}{2}} \sin\varphi, \tag{35}$$

where $0 \leq t \leq \infty$ and $0 \leq \varphi \leq 2\pi$. The Jacobian of this transformation is

$$\frac{\partial(x_1, x_2)}{\partial(t, \varphi)} = \frac{(a_1a_2)^2 ht}{(a_1^2 + t^2)^{\frac{1}{2}}(a_2^2 + t^2)^{\frac{1}{2}}}, \tag{36}$$

where

$$h = (a_1^2 + t^2)^{-1} \cos^2\varphi + (a_2^2 + t^2)^{-1} \sin^2\varphi. \tag{37}$$

In terms of these variables, we have (on S^+)

$$p = a_3(a_3^2 + t^2)^{-\frac{1}{2}}h^{-\frac{1}{2}}, \tag{38}$$

$$x_3 = a_3h^{-\frac{1}{2}}t, \tag{39}$$

$$n_1^2 = a_3^2(a_1^2 + t^2)^{-1}(a_3^2 + t^2)^{-1}h^{-1} \cos^2\varphi, \tag{40}$$

$$n_2^2 = a_3^2(a_2^2 + t^2)^{-1}(a_3^2 + t^2)^{-1}h^{-1} \sin^2\varphi, \tag{41}$$

$$n_3^2 = (a_3^2 + t^2)^{-1}t^2, \tag{42}$$

$$dS = (a_1a_2)^2(a_3^2 + t^2)h\Delta^{-1}\, dt\, d\varphi, \tag{43}$$

where Δ is given by Eq. (4).

With this transformation the φ integration in all subsequent integrals becomes elementary.

IV. SURFACE-ENERGY TENSOR $\mathcal{S}_{ij}$

The expression

$$\mathcal{S}_{ij} = \tfrac{1}{2}T \int_S (\delta_{ij} - n_in_j)\, dS \tag{44}$$

was derived in Ref. 1. This tensor is diagonal for ellipsoidal surfaces; it has components of the form

$$\mathcal{S}_{ii} = \tfrac{1}{2}T\left[\mathfrak{A}\delta_{ii} - \int_S n_i^2\, dS\right]. \tag{45}$$

In view of Eq. (43) and the definitions of the one-index symbols, the surface area $\mathfrak{A}$ becomes

$$\begin{aligned}\mathfrak{A} &= 2(a_1a_2)^2 \int_0^\infty \frac{dt}{\Delta}(a_3^2 + t^2) \int_0^{2\pi} h\, d\varphi \\ &= 2\pi(a_1a_2)^2 \int_0^\infty \frac{dt}{\Delta}\left[\frac{a_3^2 + t^2}{a_1^2 + t^2} + \frac{a_3^2 + t^2}{a_2^2 + t^2}\right] \\ &= 2\pi(a_1a_2)^2[a_3^2(\mathfrak{A}_1 + \mathfrak{A}_2) + \mathfrak{B}_1 + \mathfrak{B}_2].\end{aligned} \tag{46}$$

By using a particular case of Eq. (11), ($i = 1$, $j = 2$, and $k = 3$), we have

$$\mathfrak{A} = 2\pi(a_1a_2a_3)^2(\mathfrak{A}_1 + \mathfrak{A}_2 + \mathfrak{A}_3). \tag{47}$$

This manifestly symmetric expression for the surface area of an ellipsoid is independent of the relative magnitudes of the semiaxes.

The integral

$$\begin{aligned}\int_S n_1^2\, dS &= 2(a_1a_2a_3)^2 \int_0^\infty \frac{dt}{\Delta(a_1^2 + t^2)} \int_0^{2\pi} \cos^2\varphi\, d\varphi \\ &= 2\pi(a_1a_2a_3)^2\mathfrak{A}_1\end{aligned} \tag{48}$$

implies that

$$\int_S n_i^2\, dS = 2\pi(a_1a_2a_3)^2\mathfrak{A}_i. \tag{49}$$

In view of Eqs. (47) and (49), we obtain from Eq. (45) the result

$$\mathcal{S}_{ii} = T(\mathfrak{A}_i + \mathfrak{A}_k) \qquad (i \neq j \neq k), \tag{50}$$

where the common factor $\pi(a_1a_2a_3)^2$ has been suppressed in writing T in Eq. (50).

The components for spheroids ($a_1 = a_2$) are

$$\mathcal{S}_{11} = \mathcal{S}_{22} = T(\mathfrak{A}_1 + \mathfrak{A}_3) \tag{51}$$

and

$$\mathcal{S}_{33} = 2T\mathfrak{A}_1, \tag{52}$$

where in this case the common factor $\pi(a_1^2a_3)^2$ has been suppressed in writing T.

V. FIRST VARIATION $\delta\mathcal{S}_{ij}$

In our subsequent investigations of stability we have need primarily of the variations of $\mathcal{S}_{ij}$ for an incompressible fluid. For this case the general expression, which was derived in Ref. 1, reduces to

$$\begin{aligned}2\delta\mathcal{S}_{ij} = &-T \int_S (\delta_{ij} + n_in_j)\left(\sum_{l,m} n_ln_m \frac{\partial\xi_l}{\partial x_m}\right) dS \\ &+ T \int_S \sum_l \left(n_i \frac{\partial\xi_l}{\partial x_j} + n_j \frac{\partial\xi_l}{\partial x_i}\right)n_l\, dS.\end{aligned} \tag{53}$$

(The additional term which must be added to this expression if the fluid is compressible is evaluated in Appendix C.)

We are interested initially in the nonradial second- and third-harmonic deformations of those equilibrium configurations which have triplanar symmetry. In view of the discussion in Appendix D concerning the choice of an appropriate Lagrangian displacement, we evaluate $\delta\mathcal{S}_{ij}$ by using the form

$$\xi_i = \sum_j L_{ij}x_j, \tag{54}$$

where the L_{ij}'s represent a set of nine unknown parameters to be determined by the virial equations.

If the initial configuration is homogeneous, it is more convenient in the virial equations to replace the $L_{i;j}$'s by the unsymmetrized virials

$$V_{i;j} \equiv \int_V \rho \xi_i x_j \, d\tau = \rho L_{i;j} a_j^2, \tag{55}$$

which were defined by Chandrasekhar and Lebovitz.[5] In writing ρ in the last form of Eq. (55), we have suppressed the common factor $4\pi a_1 a_2 a_3/15$.

With this choice for ξ, we have

$$\sum_l \left(n_l \frac{\partial \xi_l}{\partial x_m} \right) = \sum_l (n_l L_{l;m}) = \rho^{-1} a_m^{-2} \sum_l (n_l V_{l;m}) \tag{56}$$

and

$$\sum_{l,m} \left(n_l n_m \frac{\partial \xi_l}{\partial x_m} \right) = \sum_{l,m} (n_l n_m L_{l;m}) = \rho^{-1} \sum_{l,m} (n_l n_m a_m^{-2} V_{l;m}). \tag{57}$$

In addition to Eq. (49), we also need the integrals

$$\int_S n_i^2 n_j^2 \, dS = 2\pi (a_1 a_2 a_3)^2 \mathfrak{B}_{ij} \qquad (i \neq j) \tag{58}$$

and

$$\int_S n_i^4 \, dS = 2\pi (a_1 a_2 a_3)^2 (3\mathfrak{B}_{ii}). \tag{59}$$

After substituting Eqs. (56) and (57) into Eq. (53), we obtain

$$2\delta \mathfrak{S}_{ij} = T \Big[L_{i;i} \int_S n_i^2 (1 - n_j^2) \, dS + L_{j;i} \int_S n_j^2 (1 - n_i^2) \, dS \Big] \qquad (i \neq j) \tag{60}$$

$$= 2T\rho^{-1} [a_i^{-2} (\mathfrak{A}_i - \mathfrak{B}_{ij}) V_{i;j} + a_i^{-2} (\mathfrak{A}_j - \mathfrak{B}_{ji}) V_{j;i}] \qquad (i \neq j) \tag{61}$$

$$= 2T\rho^{-1} \mathfrak{A}_{ij} V_{ij} \qquad (i \neq j) \tag{62}$$

and

$$2\delta \mathfrak{S}_{ii} = T \Big[L_{i;i} \int_S n_i^2 (1 - n_i^2) \, dS - L_{j;i} \int_S n_j^2 (1 + n_i^2) \, dS - L_{k;k} \int_S n_k^2 (1 + n_i^2) \, dS \Big] \qquad (i \neq j \neq k) \tag{63}$$

$$= T\rho^{-1} [a_i^{-2} (\mathfrak{A}_i - 3\mathfrak{B}_{ii}) V_{ii} - a_j^{-2} (\mathfrak{A}_j + \mathfrak{B}_{ji}) V_{ji} - a_k^{-2} (\mathfrak{A}_k + \mathfrak{B}_{ki}) V_{kk}] \quad (i \neq j \neq k), \tag{64}$$

where

$$V_{ij} = V_{i;j} + V_{j;i} \tag{65}$$

is the symmetrized virial. We have suppressed the common factor $15 a_1 a_2 a_3/4$ in writing $T\rho^{-1}$ in Eqs. (61), (62), and (64).

We give explicitly the components of $\delta \mathfrak{S}_{ij}$ for spheroids ($a_1 = a_2$) which follow from Eqs. (62) and (64):

$$2\delta \mathfrak{S}_{12} = 2\delta \mathfrak{S}_{21} = 2T\rho^{-1} \mathfrak{A}_{11} V_{12}, \tag{66}$$

$$2\delta \mathfrak{S}_{13} = 2\delta \mathfrak{S}_{31} = 2T\rho^{-1} \mathfrak{A}_{13} V_{13}, \tag{67}$$

$$2\delta \mathfrak{S}_{23} = 2\delta \mathfrak{S}_{32} = 2T\rho^{-1} \mathfrak{A}_{13} V_{23}, \tag{68}$$

$$2(\delta \mathfrak{S}_{11} - \delta \mathfrak{S}_{22}) = 2T\rho^{-1} \mathfrak{A}_{11} (V_{11} - V_{22}), \tag{69}$$

$$2(\delta \mathfrak{S}_{11} + \delta \mathfrak{S}_{22}) = -2T\rho^{-1} [2a_1^{-2} \mathfrak{B}_{11} (V_{11} + V_{22}) + a_3^{-2} (\mathfrak{A}_3 + \mathfrak{B}_{31}) V_{33}], \tag{70}$$

$$2\delta \mathfrak{S}_{33} = -T\rho^{-1} [a_1^{-2} (\mathfrak{A}_1 + \mathfrak{B}_{13}) (V_{11} + V_{22}) - a_3^{-2} (\mathfrak{A}_3 - 3\mathfrak{B}_{33}) V_{33}], \tag{71}$$

where in this case the common factor $15 a_1^2 a_3/4$ has been suppressed.

Equations (62), (64), and (66)–(71) are appropriate for an investigation of the stability of an incompressible fluid which is initially homogeneous and which is bounded by an ellipsoidal or spheroidal surface.

VI. THE THIRD-ORDER TENSORS $\mathfrak{S}_{ij;k}$ AND $\delta \mathfrak{S}_{ij;k}$

The surface-energy tensor of the third order is

$$\mathfrak{S}_{ij;k} = \tfrac{1}{2} T \int_S (\delta_{ij} - n_i n_j) x_k \, dS. \tag{72}$$

For surfaces which have triplanar symmetry, this tensor is an odd function and, therefore, vanishes.

For an incompressible fluid, the expression for the first variation of $\mathfrak{S}_{ij;k}$, which was derived in Ref. 1, reduces to

$$2\delta \mathfrak{S}_{ij;k} = T \int_S (\delta_{ij} - n_i n_j) \xi_k \, dS - T \int_S (\delta_{ij} + n_i n_j) \Big(\sum_{l,m} n_l n_m \frac{\partial \xi_l}{\partial x_m} \Big) x_k \, dS + T \int_S \sum_l \Big(n_i \frac{\partial \xi_l}{\partial} + n_j \frac{\partial \xi_l}{\partial x_i} \Big) n_l x_k \, dS. \tag{73}$$

[5] Cf. Ref. 2.

(The additional term which must be added to this expression if the fluid is compressible is evaluated in Appendix C.)

In view of the discussion in Appendix D concerning the choice of an appropriate displacement, we evaluate $\delta\mathfrak{S}_{ij;k}$ by using the form

$$\xi_i = L_i + \sum_{j,k} L_{i;jk}x_jx_k, \tag{74}$$

where the 3 L_i's and the 18 $L_{i;jk}$'s ($L_{i;jk} = L_{i;kj}$) represent a total of 21 unknown parameters to be determined by the virial equations. If the initial configuration is homogeneous, it is more convenient in the virial equations to replace these parameters by the virials

$$V_i = \int_V \rho\xi_i\, d\tau \tag{75}$$

and

$$V_{i;jk} = \int_V \rho\xi_i x_j x_k\, d\tau. \tag{76}$$

By inverting Eqs. (75) and (76), we can express the parameters in terms of the virials:

$$\tfrac{4}{7}\rho L_{i;ii}a_i^2 = 3a_i^{-2}V_{i;ii} + a_j^{-2}V_{i;jj} + a_k^{-2}V_{i;kk} - V_i \qquad (i \neq j \neq k), \tag{77}$$

$$\tfrac{4}{7}\rho L_{i;jj}a_j^2 = a_i^{-2}V_{i;ii} + 3a_j^{-2}V_{i;jj} + a_k^{-2}V_{i;kk} - V_i \qquad (i \neq j \neq k), \tag{78}$$

$$\tfrac{2}{7}\rho L_{i;ji}a_j^2a_i^2 = V_{i;ji} \qquad (i \neq j), \tag{79}$$

$$\tfrac{2}{7}\rho L_{i;jk}a_j^2a_k^2 = V_{i;jk} \qquad (i \neq j = k), \tag{80}$$

and

$$\tfrac{4}{7}\rho L_i = -a_i^{-2}V_{i;ii} - a_j^{-2}V_{i;jj} - a_k^{-2}V_{i;kk} + \tfrac{5}{7}V_i \qquad (i \neq j \neq k), \tag{81}$$

where the common factor $4\pi a_1a_2a_3/15$ has been suppressed in writing ρ in Eqs. (77)–(81).

The following integrals are needed:

$$\int_S x_i^2\, dS = \alpha a_i^4(3\mathfrak{A}_{ii} + \mathfrak{A}_{ij} + \mathfrak{A}_{ik}), \tag{82}$$

$$\int_S n_i^2x_j^2\, dS = \alpha a_i^4\mathfrak{A}_{ij} \qquad (i \neq j), \tag{83}$$

$$\int_S n_i^2x_i^2\, dS = 3\alpha a_i^4\mathfrak{A}_{ii}, \tag{84}$$

$$\int_S n_i^2n_j^2x_k^2\, dS = \alpha a_k^4\mathfrak{B}_{ijk} \qquad (i \neq j \neq k), \tag{85}$$

$$\int_S n_i^2n_j^2x_i^2\, dS = 3\alpha a_i^4\mathfrak{B}_{iji} \qquad (i \neq j), \tag{86}$$

$$\int_S n_i^4x_j^2\, dS = 3\alpha a_i^4\mathfrak{B}_{iij} \qquad (i \neq j), \tag{87}$$

$$\int_S n_i^4x_i^2\, dS = 15\alpha a_i^4\mathfrak{B}_{iii}, \tag{88}$$

$$\int_S (n_ix_i)(n_jx_j)\, dS = \alpha a_i^2a_j^2\mathfrak{A}_{ij} \qquad (i \neq j), \tag{89}$$

$$\int_S (n_ix_i)(n_jx_j)n_k^2\, dS = \alpha a_i^2a_j^2\mathfrak{B}_{ijk} \qquad (i \neq j \neq k), \tag{90}$$

and

$$\int_S (n_ix_i)(n_jx_j)n_j^2\, dS = 3\alpha a_i^2a_j^2\mathfrak{B}_{iij} \qquad (i \neq j), \tag{91}$$

where

$$\alpha = \tfrac{1}{2}\pi(a_1a_2a_3)^2. \tag{92}$$

After Eqs. (74)–(92) are substituted into Eq. (73), one finds that the resulting expressions can be written in terms of the completely symmetrized third-order virials

$$V_{ijk} \equiv V_{i;jk} + V_{j;ki} + V_{k;ij} \tag{93}$$

together with the first-order virials V_i. We have

$$2\delta\mathfrak{S}_{ij;k} = 2(\mathfrak{A}_{ij} - 2\mathfrak{B}_{ijk})V_{ijk} \qquad (i \neq j \neq k), \tag{94}$$

$$2\delta\mathfrak{S}_{ij;j} = a_i^2(\mathfrak{A}_{ji} - 2\mathfrak{B}_{jii})(a_i^{-2}V_{iii}) + 3a_j^2(\mathfrak{A}_{ji} - 2\mathfrak{B}_{jii})(a_j^{-2}V_{iij}) + a_i^2(\mathfrak{A}_{ji} - 2\mathfrak{B}_{jik})(a_k^{-2}V_{ikk}) - a_i^2\mathfrak{A}_{ji}V_i \qquad (i \neq j \neq k), \tag{95}$$

$$2\delta\mathfrak{S}_{ji;i} = -2a_i^2(\mathfrak{A}_{ii} + \mathfrak{B}_{iij})(a_i^{-2}V_{iii}) + [a_i^2(\mathfrak{A}_{ij} - 3\mathfrak{B}_{iji}) - a_j^2(\mathfrak{A}_{ji} + 3\mathfrak{B}_{jii})](a_j^{-2}V_{iij}) - (a_i^2 + a_k^2)(\mathfrak{A}_{ik} + \mathfrak{B}_{iki})(a_k^{-2}V_{ikk}) + [\mathfrak{A}_i + \mathfrak{B}_{ij} + \tfrac{3}{7}(\mathfrak{A}_i + \mathfrak{A}_k)]V_i \quad (i \neq j \neq k), \tag{96}$$

and

$$2\delta\mathfrak{S}_{ii;i} = 2a_i^2(\mathfrak{A}_{ii} - 5\mathfrak{B}_{iii})(a_i^{-2}V_{iii}) + [a_i^2(\mathfrak{A}_{ji} - 3\mathfrak{B}_{jii}) - a_j^2(\mathfrak{A}_{ij} + 3\mathfrak{B}_{iij})](a_j^{-2}V_{iij}) + [a_k^2(\mathfrak{A}_{ki} - 3\mathfrak{B}_{kii}) - a_i^2(\mathfrak{A}_{ik} + 3\mathfrak{B}_{iik})](a_k^{-2}V_{ikk}) + [3\mathfrak{B}_{ii} - \mathfrak{A}_i + \tfrac{3}{7}(\mathfrak{A}_j + \mathfrak{A}_k)]V_i \qquad (i \neq j \neq k), \tag{97}$$

where the common factor $(7T/4\rho)(15a_1a_2a_3/4)$ has been suppressed in writing Eqs. (94)–(97). Equations (94)–(97) are appropriate for an investigation of the stability of an incompressible fluid which is bounded by an ellipsoidal surface.

TABLE I. The coefficients of the virials in the expansions of $\delta\mathfrak{S}_{ij;k}$ for ellipsoids. The common factor $(7T/4\rho)(15a_1a_2a_3/4)$ has been suppressed in each coefficient.

	$a_1^{-2}V_{111}$	$a_2^{-2}V_{122}$	$a_3^{-2}V_{133}$
$2\delta\mathfrak{S}_{11;1}$	$2a_1^2(\mathfrak{a}_{11} - 5\mathfrak{B}_{111})$	$a_2^2(\mathfrak{a}_{21} - 3\mathfrak{B}_{211}) - a_1^2(\mathfrak{a}_{12} + 3\mathfrak{B}_{112})$	$a_3^2(\mathfrak{a}_{31} - 3\mathfrak{B}_{311}) - a_1^2(\mathfrak{a}_{13} + 3\mathfrak{B}_{113})$
$2\delta\mathfrak{S}_{22;1}$	$-2a_1^2(\mathfrak{a}_{11} + \mathfrak{B}_{112})$	$a_1^2(\mathfrak{a}_{12} - 3\mathfrak{B}_{122}) - a_2^2(\mathfrak{a}_{21} + 3\mathfrak{B}_{221})$	$-(a_1^2 + a_3^2)(\mathfrak{a}_{13} + \mathfrak{B}_{132})$
$2\delta\mathfrak{S}_{33;1}$	$-2a_1^2(\mathfrak{a}_{11} + \mathfrak{B}_{113})$	$-(a_1^2 + a_2^2)(\mathfrak{a}_{12} + \mathfrak{B}_{123})$	$a_1^2(\mathfrak{a}_{13} - 3\mathfrak{B}_{133}) - a_3^2(\mathfrak{a}_{31} + 3\mathfrak{B}_{331})$
$2\delta\mathfrak{S}_{12;2}$	$a_2^2(\mathfrak{a}_{21} - 2\mathfrak{B}_{211})$	$3a_2^2(\mathfrak{a}_{21} - 2\mathfrak{B}_{221})$	$a_2^2(\mathfrak{a}_{21} - 2\mathfrak{B}_{213})$
$2\delta\mathfrak{S}_{13;3}$	$a_3^2(\mathfrak{a}_{31} - 2\mathfrak{B}_{311})$	$a_3^2(\mathfrak{a}_{31} - 2\mathfrak{B}_{312})$	$3a_3^2(\mathfrak{a}_{31} - 2\mathfrak{B}_{331})$
	$a_2^{-2}V_{222}$	$a_1^{-2}V_{211}$	$a_3^{-2}V_{233}$
$2\delta\mathfrak{S}_{22;2}$	$2a_2^2(\mathfrak{a}_{22} - 5\mathfrak{B}_{222})$	$a_1^2(\mathfrak{a}_{12} - 3\mathfrak{B}_{122}) - a_2^2(\mathfrak{a}_{21} + 3\mathfrak{B}_{221})$	$a_3^2(\mathfrak{a}_{32} - 3\mathfrak{B}_{322}) - a_2^2(\mathfrak{a}_{23} + 3\mathfrak{B}_{223})$
$2\delta\mathfrak{S}_{11;2}$	$-2a_2^2(\mathfrak{a}_{22} + \mathfrak{B}_{221})$	$a_2^2(\mathfrak{a}_{21} - 3\mathfrak{B}_{211}) - a_1^2(\mathfrak{a}_{12} + 3\mathfrak{B}_{112})$	$-(a_2^2 + a_3^2)(\mathfrak{a}_{23} + \mathfrak{B}_{231})$
$2\delta\mathfrak{S}_{33;2}$	$2a_2^2(\mathfrak{a}_{22} + \mathfrak{B}_{223})$	$-(a_2^2 + a_1^2)(\mathfrak{a}_{21} + \mathfrak{B}_{213})$	$a_2^2(\mathfrak{a}_{23} - 3\mathfrak{B}_{233}) - a_3^2(\mathfrak{a}_{32} + 3\mathfrak{B}_{332})$
$2\delta\mathfrak{S}_{21;1}$	$a_1^2(\mathfrak{a}_{12} - 2\mathfrak{B}_{122})$	$3a_1^2(\mathfrak{a}_{12} - 2\mathfrak{B}_{112})$	$a_1^2(\mathfrak{a}_{12} - 2\mathfrak{B}_{123})$
$2\delta\mathfrak{S}_{23;3}$	$a_3^2(\mathfrak{a}_{32} - 2\mathfrak{B}_{322})$	$a_3^2(\mathfrak{a}_{32} - 2\mathfrak{B}_{321})$	$3a_3^2(\mathfrak{a}_{32} - 2\mathfrak{B}_{332})$
	$a_3^{-2}V_{333}$	$a_2^{-2}V_{322}$	$a_1^{-2}V_{311}$
$2\delta\mathfrak{S}_{33;3}$	$2a_3^2(\mathfrak{a}_{33} - 5\mathfrak{B}_{333})$	$a_2^2(\mathfrak{a}_{23} - 3\mathfrak{B}_{233}) - a_3^2(\mathfrak{a}_{32} + 3\mathfrak{B}_{332})$	$a_1^2(\mathfrak{a}_{13} - 3\mathfrak{B}_{133}) - a_3^2(\mathfrak{a}_{31} + 3\mathfrak{B}_{331})$
$2\delta\mathfrak{S}_{22;3}$	$-2a_3^2(\mathfrak{a}_{33} + \mathfrak{B}_{332})$	$a_3^2(\mathfrak{a}_{32} - 3\mathfrak{B}_{322}) - a_2^2(\mathfrak{a}_{23} + 3\mathfrak{B}_{223})$	$-(a_3^2 + a_1^2)(\mathfrak{a}_{31} + \mathfrak{B}_{312})$
$2\delta\mathfrak{S}_{11;3}$	$-2a_3^2(\mathfrak{a}_{33} + \mathfrak{B}_{331})$	$-(a_3^2 + a_2^2)(\mathfrak{a}_{32} + \mathfrak{B}_{321})$	$a_3^2(\mathfrak{a}_{31} - 3\mathfrak{B}_{311}) - a_1^2(\mathfrak{a}_{13} + 3\mathfrak{B}_{113})$
$2\delta\mathfrak{S}_{32;2}$	$a_2^2(\mathfrak{a}_{23} - 2\mathfrak{B}_{233})$	$3a_2^2(\mathfrak{a}_{23} - 2\mathfrak{B}_{223})$	$a_2^2(\mathfrak{a}_{23} - 2\mathfrak{B}_{231})$
$2\delta\mathfrak{S}_{31;1}$	$a_1^2(\mathfrak{a}_{13} - 2\mathfrak{B}_{133})$	$a_1^2(\mathfrak{a}_{13} - 2\mathfrak{B}_{132})$	$3a_1^2(\mathfrak{a}_{13} - 2\mathfrak{B}_{113})$

If the Lagrangian displacement is referred in a frame in which the center of mass of the fluid is at rest, then we can set

$$V_i \equiv 0 \tag{98}$$

without any loss in generality.

In working with Eqs. (95)–(97) it is convenient to have in explicit form the coefficients of the virials in the different $\delta\mathfrak{S}_{ij;k}$'s. Table I provides these coefficients for ellipsoids, and Table II provides these coefficients for spheroids ($a_1 = a_2$). Table I is to be compared with the corresponding table obtained by Chandrasekhar and Lebovitz[6] for $\delta\mathfrak{W}_{ij;k}$ in the theory of gravitation.

TABLE II. The coefficients of the virials in the expansions of $\delta\mathfrak{S}_{ij;k}$ for spheroids ($a_1 = a_2$). The common factor $(7T/4\rho)(15a_1^2a_3/4)$ has been suppressed in each coefficient.

	$a_1^{-2}V_{111}$ $(a_1^{-2}V_{222})$	$a_1^{-2}V_{122}$ $(a_1^{-2}V_{211})$	$a_3^{-2}V_{133}$ $(a_3^{-2}V_{233})$
$2\delta\mathfrak{S}_{11;1}$ $(2\delta\mathfrak{S}_{22;2})$	$2a_1^2(\mathfrak{a}_{11} - 5\mathfrak{B}_{111})$	$-6a_1^2\mathfrak{B}_{111}$	$a_3^2(\mathfrak{a}_{31} - 3\mathfrak{B}_{311}) - a_1^2(\mathfrak{a}_{13} + 3\mathfrak{B}_{113})$
$2\delta\mathfrak{S}_{22;1}$ $(2\delta\mathfrak{S}_{11;2})$	$-2a_1^2(\mathfrak{a}_{11} + \mathfrak{B}_{111})$	$-6a_1^2\mathfrak{B}_{111}$	$-(a_1^2 + a_3^2)(\mathfrak{a}_{13} + \mathfrak{B}_{131})$
$2\delta\mathfrak{S}_{33;1}$ $(2\delta\mathfrak{S}_{33;2})$	$-2a_1^2(\mathfrak{a}_{11} + \mathfrak{B}_{113})$	$-2a_1^2(\mathfrak{a}_{11} + \mathfrak{B}_{113})$	$a_1^2(\mathfrak{a}_{13} - 3\mathfrak{B}_{133}) - a_3^2(\mathfrak{a}_{31} + 3\mathfrak{B}_{331})$
$2\delta\mathfrak{S}_{12;2}$ $(2\delta\mathfrak{S}_{21;1})$	$a_1^2(\mathfrak{a}_{11} - 2\mathfrak{B}_{111})$	$3a_1^2(\mathfrak{a}_{11} - 2\mathfrak{B}_{111})$	$a_1^2(\mathfrak{a}_{11} - 2\mathfrak{B}_{113})$
$2\delta\mathfrak{S}_{13;3}$ $(2\delta\mathfrak{S}_{23;3})$	$a_3^2(\mathfrak{a}_{31} - 2\mathfrak{B}_{311})$	$a_3^2(\mathfrak{a}_{31} - 2\mathfrak{B}_{311})$	$3a_3^2(\mathfrak{a}_{31} - 2\mathfrak{B}_{331})$
	$a_3^{-2}V_{333}$	$a_1^{-2}(V_{311} + V_{322})$	$a_1^{-2}(V_{311} - V_{322})$
$2\delta\mathfrak{S}_{33;3}$	$2a_3^2(\mathfrak{a}_{33} - 5\mathfrak{B}_{333})$	$a_1^2(\mathfrak{a}_{13} - 3\mathfrak{B}_{133}) - a_3^2(\mathfrak{a}_{31} + 3\mathfrak{B}_{331})$	0
$2(\delta\mathfrak{S}_{11;3} + \delta\mathfrak{S}_{22;3})$	$-4a_3^2(\mathfrak{a}_{33} + \mathfrak{B}_{331})$	$-2a_1^2(\mathfrak{a}_{13} + 2\mathfrak{B}_{113}) - 4a_3^2\mathfrak{B}_{311}$	0
$2(\delta\mathfrak{S}_{31;1} + \delta\mathfrak{S}_{32;2})$	$2a_1^2(\mathfrak{a}_{13} - 2\mathfrak{B}_{133})$	$4a_1^2(\mathfrak{a}_{13} - 2\mathfrak{B}_{113})$	0
$2(\delta\mathfrak{S}_{11;3} - \delta\mathfrak{S}_{22;3})$	0	0	$2a_1^2(\mathfrak{a}_{11} - 2\mathfrak{B}_{113})$
$2(\delta\mathfrak{S}_{31;1} - \delta\mathfrak{S}_{32;2})$	0	0	$2a_1^2(\mathfrak{a}_{13} - 2\mathfrak{B}_{113})$

[6] S. Chandrasekhar and N. R. Lebovitz, Astrophys. J. 137, 1142 (1963), Table 1.

VII. CONCLUDING REMARKS

In this paper the surface-energy tensors have been evaluated for ellipsoidal surfaces. The final expressions have been given in terms of particular types of elliptic integrals which may be numerically evaluated using the algebraic recursion relations derived in Sec. II.

In subsequent papers we shall make use of these formulas in an investigation of the stability of a rotating uniformly charged homogeneous liquid drop (held together by a constant surface tension) using the method of the tensor virial.

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APPENDIX A. EVALUATION OF $\mathcal{A}_1$, $\mathcal{A}_2$, AND $\mathcal{A}_3$

The integrals defining the $\mathcal{A}_i$'s can be expressed in terms of the incomplete elliptic integrals

$$F(\theta, \phi) = \int_0^{\phi} (1 - \sin^2\theta \sin^2\varphi)^{-\frac{1}{2}}\, d\varphi \tag{A1}$$

and

$$E(\theta, \phi) = \int_0^{\phi} (1 - \sin^2\theta \sin^2\varphi)^{\frac{1}{2}}\, d\varphi, \tag{A2}$$

where

$$\sin\theta = \frac{a_1}{a_2}\left(\frac{a_2^2 - a_3^2}{a_1^2 - a_3^2}\right)^{\frac{1}{2}} \quad \text{and} \quad \cos\phi = \frac{a_3}{a_1}. \tag{A3}$$

Assume that $a_1 > a_2 > a_3$, and let

$$t = a_3(\sin^2\phi - \sin^2\varphi)^{-\frac{1}{2}} \sin\varphi \tag{A4}$$

in Eq. (5). Then

$$\mathcal{A}_1 = (a_1^3 a_2 \sin^3\phi \cos^2\theta)^{-1}[\sin^2\phi \cos^2\theta\, F(\theta, \phi) + \cos^2\phi\, E(\theta, \phi) - (a_3/a_2)\sin\phi\cos\phi], \tag{A5}$$

$$\mathcal{A}_2 = (a_1 a_2^3 \sin^3\phi \sin^2\theta \cos^2\theta)^{-1}[\cos^2\theta\, F(\theta, \phi) - (a_3^2/a_2^2)E(\theta, \phi) + (a_3/a_2)\sin\phi\cos\phi\sin^2\theta], \tag{A6}$$

and

$$\mathcal{A}_3 = (a_1 a_2 a_3^2 \sin^3\phi \sin^2\theta)^{-1} \times [E(\theta, \phi) - (a_3^2/a_2^2)F(\theta, \phi)]. \tag{A7}$$

When $a_1 = a_2$, the integrals defining the $\mathcal{A}_i$'s become elementary. For prolate spheroids ($a_1 = a_2 < a_3$), we have

$$\mathcal{A}_1 = \mathcal{A}_2 = \frac{(1 - k^2)^{\frac{1}{2}}}{2a_1^4 k^2} \times \left[(1 - k^2)^{\frac{1}{2}} - (1 - 2k^2)\frac{\sin^{-1} k}{k}\right] \tag{A8}$$

and

$$\mathcal{A}_3 = \frac{(1 - k^2)^{-\frac{1}{2}}}{a_3^4 k^2}\left[\frac{\sin^{-1} k}{k} - (1 - k^2)^{\frac{1}{2}}\right], \tag{A9}$$

where

$$k^2 = 1 - (a_1^2/a_3^2). \tag{A10}$$

For oblate spheroids ($a_1 = a_2 > a_3$), we have

$$\mathcal{A}_1 = \mathcal{A}_2 = (2a_1^4 e^2)^{-1} \times [(1 + e^2)(\tanh^{-1} e)/e - 1] \tag{A11}$$

and

$$\mathcal{A}_3 = (a_1^4 e^2)^{-1}[(1 - e^2)^{-1} - (\tanh^{-1} e)/e], \tag{A12}$$

where

$$e^2 = 1 - (a_3^2/a_1^2). \tag{A13}$$

APPENDIX B. A RECIPROCAL RELATIONSHIP

The multi-index symbols for the potentials and superpotentials of homogeneous ellipsoids were defined by Chandrasekhar and Lebovitz in Ref. 3. Our multi-index symbols for the surface energy of an ellipsoid with semi-axes (a_1, a_2, a_3) are closely related to the multi-index symbols for the potential of the corresponding *reciprocal* ellipsoid with semi-axes $(a_1^{-1}, a_2^{-1}, a_3^{-1})$. Denote the functional dependence of the integrals on the semiaxes as q for the ellipsoid and as q^{-1} for the reciprocal ellipsoid. Then by letting

$$t = u^{-\frac{1}{2}} \tag{B1}$$

in Eq. (1), one obtains

$$(2a_1 a_2 a_3)\mathcal{I}(q) = I(q^{-1}) \equiv \int_0^{\infty} \frac{du}{\Delta(q^{-1}, u)}, \tag{B2}$$

where

$$\Delta^2(q^{-1}, u) = (a_1^{-2} + u)(a_2^{-2} + u)(a_3^{-2} + u). \tag{B3}$$

The integral $I(q)$ is related to the potential at the origin and to the potential energy of the ellipsoid. The geometrical meaning of $\mathcal{I}(q)$ follows from the relation

$$4\pi(a_1 a_2 a_3)^2 \mathcal{I}(q) = \int_S p^2\, dS, \tag{B4}$$

where p [given by Eq. (33)] is the distance from the origin to the tangent plane which passes through

the point (x_1, x_2, x_3) on the surface of the ellipsoid.

Similarly, one can show, for example, that

$$(2a_1a_2a_3)a_i^2\mathfrak{A}_i(q) = B_i(q^{-1}), \tag{B5}$$

$$(2a_1a_2a_3)a_i^2\mathfrak{B}_i(q) = A_i(q^{-1}), \tag{B6}$$

and

$$(2a_1a_2a_3)a_i^2a_j^2\mathfrak{A}_{ij}(q) = B_i(q^{-1}) - a_j^{-2}B_{ji}(q^{-1}) \tag{B7}$$

$$= B_j(q^{-1}) - a_i^{-2}B_{ij}(q^{-1}), \tag{B8}$$

where A_i, B_i, and B_{ij} are multi-index symbols for the potential which are defined in Ref. 3.

Unfortunately, Eqs. (B5)–(B8) are not of practical use in computing the $\mathfrak{A}_i$'s because existing tables[7] of the A_i's do not cover the appropriate range.

APPENDIX C. CORRECTIONS DUE TO COMPRESSIBILITY

In Secs. V and VI the variations $\delta\mathfrak{S}_{ij}$ and $\delta\mathfrak{S}_{ij;k}$ were evaluated for an incompressible fluid. Here, we evaluate the terms [derived in Ref. 1] which must be added to Eqs. (53) and (73) when the fluid is compressible.

We must add to the general expression for $2\delta\mathfrak{S}_{ij}$ in Eq. (53) the quantity

$$T\int_S (\delta_{ij} - n_in_j)\,\mathrm{div}\,\xi\,dS. \tag{C1}$$

This affects only the diagonal terms $2\delta\mathfrak{S}_{ii}$ given by Eq. (63). To Eq. (63) we must add the quantity

$$T(L_{i;i} + L_{j;i} + L_{k;k})\int_S (1 - n_i^2)\,dS \qquad (i \neq j \neq k), \tag{C2}$$

which has the value

$$2T(L_{i;i} + L_{j;j} + L_{k;k})(\mathfrak{A}_j + \mathfrak{A}_k) \qquad (i \neq j \neq k) \tag{C3}$$

for ellipsoids. If the initial configuration is homogeneous, we may use the relation

$$2\rho(L_{i;i} + L_{j;j} + L_{k;k}) = a_i^{-2}V_{ii} + a_j^{-2}V_{ij} + a_k^{-2}V_{kk} \tag{C4}$$

in (C3) to obtain the correction to Eq. (64).

We must add to the general expression for $2\delta\mathfrak{S}_{ij;k}$ given by Eq. (73) the quantity

$$T\int_S (\delta_{ij} - n_in_j)x_k\,\mathrm{div}\,\xi\,dS. \tag{C5}$$

For ellipsoids this contributes to $2\delta\mathfrak{S}_{ij;j}$ the quantity

$$-T(L_{i;ii} + L_{j;ij} + L_{k;ik})a_i^2a_j^2\mathfrak{A}_{ij} \qquad (i \neq j \neq k), \tag{C6}$$

to $2\delta\mathfrak{S}_{jj;i}$ the quantity

$$T(L_{i;ii} + L_{j;ij} + L_{k;ik})a_i^4(3\mathfrak{A}_{ii} + \mathfrak{A}_{ik}) \qquad (i \neq j \neq k), \tag{C7}$$

and to $2\delta\mathfrak{S}_{ii;i}$ the quantity

$$T(L_{i;ii} + L_{j;ij} + L_{k;ik})a_i^4(\mathfrak{A}_{ij} + \mathfrak{A}_{ik}) \qquad (i \neq j \neq k). \tag{C8}$$

If the initial configuration is homogeneous, the relation

$$4\rho a_i^2(L_{i;ii} + L_{j;ij} + L_{k;ik}) = 7(a_i^{-2}V_{iii} + a_j^{-2}V_{ijj} + a_k^{-2}V_{ikk} - V_i) \tag{C9}$$

may be used in (C6)–(C8) to obtain the corrections to Eqs. (95)–(97).

We have suppressed the factor $\pi(a_1a_2a_3)^2$ in writing T in (C3) and (C6)–(C8), and we have suppressed the factor $4\pi a_1a_2a_3/15$ in writing ρ in Eqs. (C4) and (C9).

APPENDIX D. VIRIAL METHOD

In the present considerations, the method of Cartesian moments or the method of the tensor virial, which has been developed by Chandrasekhar and Lebovitz,[2] is used to investigate the equilibrium and the stability of a freely moving classical system. The set of all virial equations is generated by taking successively higher moments (with respect to the Cartesian coordinates) of the components of the equation governing the motion of the system. The zeroth moments provide three integral relations; the first moments provide nine additional integral relations; the second moments provide eighteen more integral relations; and in general, the mth moments provide

$$N_m = \tfrac{1}{2}(m^2 + 3m + 2), \quad m = 0, 1, 2, \cdots \tag{D1}$$

integral relations which must be satisfied by the system. When written in tensor form, the set of N_m equations provided by the mth moments comprises the *tensor virial theorem* of order $m + 1$.

These tensor virial theorems provide the basis for an investigation of the equilibrium and the stability of the system. Each tensor component of the virial theorems (i.e., each moment equation) provides an *exact* integral relation which must be satisfied by the system under any conditions compatible with the initially assumed equation of motion. In par-

[7] S. Chandrasekhar, Astrophys. J. **136**, 1048 (1962).

ticular, these relations must be satisfied when the motion of the system is in a steady state and equilibrium prevails. In addition, the first variation of each tensor component of the virial theorems provides an exact integral relation which must be satisfied in all cases of infinitesimal perturbations, and in particular, these relations must be satisfied by the proper solutions belonging to the natural modes of oscillation of the system.

In subsequent papers we shall use the virial equations to investigate the equilibrium and the stability of a rotating uniformly-charged incompressible liquid drop held together by a constant surface tension. Due to the presence of the surface tension, the figures of equilibrium which have triplanar symmetry are not exactly spheroids nor ellipsoids. Nevertheless, we show in a subsequent paper that all of the equilibrium relations, provided by the virial equations through the third order, can be satisfied by *assuming* that the figures of equilibrium are ellipsoids. With these assumed shapes, we are justified in investigating the stability with respect to second- and third-harmonic deformations of those equilibrium configurations which have triplanar symmetry. This assumption about the shape cannot be greatly in error so long as the rate of rotation is slow enough that the exact figures of equilibrium have not yet developed a dimple in the polar regions or an equatorial constriction. (The limits under which this assumption is valid will be given in a subsequent paper.)

We obtain the natural, nonradial modes of oscillation of a rotating charged liquid drop by using the first variations of the virial theorems. Since the solutions belonging to the natural modes of oscillation will have a time dependence of the form

$$e^{\lambda t}, \tag{D2}$$

where λ is a parameter whose characteristic values are to be determined; we choose the Lagrangian displacement to have the form

$$\xi(\mathbf{x})e^{\lambda t}. \tag{D3}$$

By inserting for the Lagrangian displacement in the virial equations, a "trial function" $\xi(\mathbf{x})$, with a space dependence which one might use, for example, in a variational treatment of this problem, we obtain a set of equations which enables us to determine the frequencies of oscillation with some precision. Clearly, we cannot use a trial function with any more unknown parameters than the total number of virial equations that we choose to consider. The simplest trial function that suggests itself in this connection has the form

$$\xi_i = L_i + \sum_j L_{i;j}x_j + \sum_{j,k} L_{i;jk}x_jx_k + \cdots, \tag{D4}$$

where the L's are unknown constants. Since i may assume the values 1 to 3, there are a total of three L_i's, nine $L_{i;j}$'s, eighteen $L_{i;jk}$'s (note that $L_{i;jk} = L_{i;kj}$, by symmetry), and in general, N_m different constants of order $m + 1$.

We can obtain the oscillation frequencies associated with the second- and third-harmonic deformations, if we terminate the series in Eq. (D4) after the terms shown and consider just the virial equations through the third order. Because of the triplanar symmetry of the assumed figures of equilibrium, the variation $\delta\mathfrak{S}_{ij}$ depends only on the terms in ξ_i which contain $L_{i;j}$'s and is independent of the L_i's and the $L_{i;jk}$'s. Thus, without loss of generality, we may evaluate $\delta\mathfrak{S}_{ij}$ by using the form of ξ_i given by Eq. (54). For the same reasons, the variation $\delta\mathfrak{S}_{ij;k}$ is independent of the $L_{i;j}$'s, so that we may evaluate $\delta\mathfrak{S}_{ij;k}$ by using ξ_i given by Eq. (74).

In choosing ξ_i to have the form given by Eq. (D4), we have been guided by the fact that this trial function leads to the *exact* proper solutions in the case of a self-gravitating mass where, moreover, ellipsoids are exact figures of equilibrium. Similar assumptions concerning ξ_i have been made by Chandrasekhar and Lebovitz in considering the oscillations and stability of rotating, gaseous masses;[8,9] and by Chandrasekhar in considering the stability of a rotating neutrally charged liquid drop.[10] This way of applying the virial method to these problems resembles the solution of a characteristic value problem by a variational method for which approximate eigenfunctions still yield moderately good eigenvalues.

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[8] S. Chandrasekhar and N. R. Lebovitz, Astrophys. J. **135**, 248 (1962).
[9] S. Chandrasekhar and N. R. Lebovitz, Astrophys. J. **138**, 185 (1963).
[10] S. Chandrasekhar, Proc. Roy. Soc. (London) **A286**, 1 (1964).

Stability of Axisymmetric Figures of Equilibrium of a Rotating Charged Liquid Drop*

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The method of the tensor virial is used to investigate the equilibrium and stability of a rotating, uniformly charged (with a total charge Q), incompressible liquid drop (of volume V) held together by a constant surface tension T. The tensor virial theorems provide relations which define the sequences of equilibrium figures and perturbation equations which govern the oscillations. Since spheroids satisfy the virial theorems of orders one, two, and three, the stability of exact axisymmetric equilibrium figures with respect to second- and third-harmonic deformations can be inferred from the nature of the characteristic oscillation frequencies of spheroids. As the rotation increases for a given fissionability parameter $x = Q^2/10TV$ $(0 \leq x < 1)$, a sequence of oblate spheroids representing initially stable rotating ground states exhibits a neutral point (where an ellipsoidal sequence bifurcates), but remains stable (in the absence of dissipation) until one of the three second-harmonic modes of vibration (the toroidal or γ mode) becomes overstable. Later, for third harmonics, it exhibits a second neutral point (where a sequence of asymmetric figures bifurcates), but again remains stable until the onset of the associated overstability. A third neutral point does not indicate the bifurcation of pear shapes. The error in using oblate spheroids is less than 5% up to the first overstable point. One class of saddle shapes can be represented by prolate spheroids (which must rotate about the symmetry axis) in the neighborhood of $x = 1$. They are initially unstable with respect to the other two second-harmonic modes of vibration (the pulsation or β mode and the transverse-shear mode).

I. INTRODUCTION

THE interpretation of heavy-ion-induced fission has revived interest in the classical problem of a rotating charged liquid drop. The theory of nuclear fission proposed by Bohr and Wheeler[1] involved equilibrium saddle shapes of a nonrotating charged liquid drop. More recent analytical and numerical investigations of these saddle shapes, and in particular, the investigations of Cohen and Swiatecki,[2,3] are summarized by Hyde[4] and Wilets.[5] The influence of angular momentum on these saddle shapes was first investigated by Pik-Pichak[6] and later by Hiskes.[7] Further investigations along these lines have been made by Beringer and Knox[8] using spheroids and by Carlson and Pao Lu[9] using ellipsoids. Extensive numerical investigations along the lines of Refs. 2 and 3 are in progress; some preliminary results have been given by Cohen, Plasil, and Swiatecki[10] and by Plasil.[11]

In this paper and in subsequent papers, we use the method of the tensor virial to investigate the equilibrium and the stability of a rotating uniformly charged incompressible liquid drop held together by a constant surface tension. The virial method was developed by Chandrasekhar,[12] and has already been applied by Chandrasekhar and Lebovitz to a wide variety of problems in the theory of self-gravitating masses. A summary of their investigations has been given by Chandrasekhar.[13]

In the virial method, the equations of motion are replaced by an infinite set of virial theorems. These virial theorems are generated by taking successively higher moments (with respect to the Cartesian coordinates) of the equations of motion.

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[1] N. Bohr and J. Wheeler, Phys. Rev. 56, 426 (1939).

[2] S. Cohen and W. J. Swiatecki, Ann. Phys. (N. Y.) 19, 67 (1962).

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[4] E. K. Hyde, *The Nuclear Properties of the Heavy Elements* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1964), Vol. III, Chap. 2.

[5] L. Wilets, *Theories of Nuclear Fission* (Clarendon Press, Oxford, England, 1964).

[6] G. A. Pik-Pichak, Zh. Eksperim. i Teor. Fiz. 34, 341 (1958) [English transl.: Soviet Phys.—JETP 7, 238 (1958)].

[7] J. R. Hiskes, University of California Lawrence Radiation Laboratory Rept. UCRL-9275 (1960).

[8] R. Beringer and W. J. Knox, Phys. Rev. 121, 1195 (1961).

[9] B. C. Carlson and Pao Lu, in *Proceedings of the Rutherford Jubilee International Conference, Manchester, 1961*, J. B. Birks, Ed. (Heywood and Company, London, 1961) p. 291.

[10] S. Cohen, F. Plasil, and W. J. Swiatecki, in *Proceedings of the Third Conference on Reactions between Complex Nuclei*, A. Ghiorso, R. M. Diamond, and H. E. Conzett, Eds. (The University of California Press, Berkeley, California, 1963), p. 325.

[11] F. Plasil, University of California Radiation Laboratory Rept. UCRL-11193 (1963).

[12] S. Chandrasekhar, *Hydrodynamic and Hydromagnetic Stability* (Clarendon Press, Oxford, England, 1961), Chap. 13.

[13] S. Chandrasekhar, in *Lectures in Theoretical Physics*, W. E. Brittin and W. R. Chappell, Eds. (The University of Colorado Press, Boulder, Colorado, 1964), Vol. VI, p. 1.

The tensor virial theorems provide a definite number of exact time-dependent integral relations in each order which must be satisfied under any conditions compatible with the initially assumed equations of motion of the fluid.

In particular, these virial relations must be satisfied when the motion of the fluid is in a steady state and hydrostatic equilibrium prevails. An exact equilibrium configuration satisfies all of the relations in every order. Conversely, these relations may be used in successive orders to place definite restrictions on the shape of any *assumed* figure of equilibrium. Due to the presence of surface tension, those exact figures of equilibrium which have triplanar symmetry are neither spheroids nor ellipsoids. Nevertheless, we show that all of the equilibrium relations, provided by the virial theorems through the third order, can be satisfied by assuming that the figures of equilibrium *are* ellipsoids. With these assumed shapes, we are justified in investigating the stability, with respect to second- and third-harmonic deformations, of those exact equilibrium configurations which have triplanar symmetry. (We shall set definite limits on the validity of this assumption.)

The first variations of the virial theorems provide exact time-dependent integral relations which must be satisfied in all cases of infinitesimal perturbations. In particular, these relations must be satisfied by the proper solutions belonging to the natural modes of oscillation. By making an appropriate choice for the form of these proper solutions, sets of equations are obtained from which the frequencies of oscillation can be determined with some precision. An examination of the character of these frequencies of oscillation leads to the conditions for the onset of instability. This aspect of the virial method resembles the solution of a characteristic value problem by a variational method for which approximate eigenfunctions still yield moderately good eigenvalues.

II. TENSOR VIRIAL THEOREMS

We describe the motion of a charged liquid drop in a frame of reference rotating with a constant angular velocity $\mathbf{\Omega}$, which is chosen to lie along x_3. In this frame of reference, the equation governing the motion of a fluid element having a mass density ρ and a positive charge density σ is

$$\rho \frac{du_i}{dt} - 2\rho\Omega\epsilon_{il3}u_l = -\frac{\partial p}{\partial x_i} - \sigma\frac{\partial \mathfrak{V}}{\partial x_i} + \rho\Omega^2(x_i - \delta_{i3}\,x_3), \tag{1}$$

where $\mathbf{u}$ is the velocity, p is the hydrostatic pressure, and

$$\mathfrak{V}(\mathbf{x}) = \int_V \frac{\sigma(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}\,d\tau' \tag{2}$$

is the electrostatic potential. (The summation convention over repeated indices applies to all the formulas in this section.)

The tensor virial theorem of the first order is obtained by integrating the ith component of the equation of motion over the volume occupied by the fluid. We have

$$\frac{d}{dt}\int_V \rho u_i\,d\tau - 2\Omega\epsilon_{il3}\int_V \rho u_l\,d\tau = \Omega^2(I_i - \delta_{i3}\,I_3), \tag{3}$$

where the quantities

$$I_i = \int_V \rho x_i\,d\tau \tag{4}$$

define the position of the center of mass.

The tensor virial theorem of the second order is obtained by first multiplying the ith component of the equation of motion by the Cartesian coordinate x_j, and then integrating the result over the volume occupied by the fluid. We have

$$\frac{d}{dt}\int_V \rho u_i x_j\,d\tau - 2\Omega\epsilon_{il3}\int_V \rho u_l x_j\,d\tau = 2\mathfrak{T}_{ij} - 2\mathfrak{S}_{ij} + \mathfrak{W}_{ij} + \Omega^2(I_{ij} - \delta_{i3}\,I_{3i}) + \Pi\,\delta_{ij}. \tag{5}$$

The kinetic-energy tensor is

$$\mathfrak{T}_{ij} = \frac{1}{2}\int_V \rho u_i u_j\,d\tau. \tag{6}$$

The surface-energy tensor is

$$\mathfrak{S}_{ij} = \tfrac{1}{2}T\int_S (\delta_{ij} - n_i n_j)\,dS, \tag{7}$$

where n_i is a component of the unit outward normal to the surface $\mathbf{S}$ and T is a constant surface tension. The transformations which lead to this definition of $\mathfrak{S}_{ij}$ are described in Ref. 14. The potential-energy tensor is

$$\mathfrak{W}_{ij} = -\int_V \sigma x_i\frac{\partial \mathfrak{V}}{\partial x_i}\,d\tau = \frac{1}{2}\int_V \sigma\mathfrak{V}_{ij}\,d\tau, \tag{8}$$

where

$$\mathfrak{V}_{ij}(\mathbf{x}) = \int_V \sigma(\mathbf{x}')\frac{(x_i - x_i')(x_j - x_j')}{|\mathbf{x} - \mathbf{x}'|^3}\,d\tau' \tag{9}$$

[14] C. E. Rosenkilde, J. Math. Phys. **8**, 84 (1967).

is the tensor potential. This potential-energy tensor is formally identical (apart from sign) with the potential-energy tensor defined by Chandrasekhar[13] for self-gravitating fluids. The tensor potential and quantities related to it have been discussed by Chandrasekhar and Lebovitz.[15,16] The moment of inertia tensor is

$$I_{ij} = \int_V \rho x_i x_j \, d\tau. \tag{10}$$

The quantity

$$\Pi = \int_V p \, d\tau \tag{11}$$

is related to the internal energy of the fluid. The trace of the tensor virial theorem of the second order reduces to the scalar form of the virial theorem.

The tensor virial theorem of the third order is obtained by first multiplying the ith component of the equation of motion by $x_j x_k$, and then integrating over the volume. We have

$$\begin{aligned}\frac{d}{dt}\int_V \rho u_i x_j x_k \, d\tau - 2\Omega\epsilon_{i\,l\,3}\int_V \rho u_l x_j x_k \, d\tau \\ = 2\mathfrak{T}_{ij;k} - 2\mathfrak{S}_{ij;k} + \mathfrak{W}_{ij;k} + \delta_{ij}\Pi_k \\ + 2\mathfrak{T}_{ik;j} - 2\mathfrak{S}_{ik;j} + \mathfrak{W}_{ik;j} + \delta_{ik}\Pi_j \\ + \Omega^2(I_{ijk} - \delta_{i3} I_{3jk}),\end{aligned} \tag{12}$$

where

$$\mathfrak{T}_{ij;k} = \frac{1}{2}\int_V \rho u_i u_j x_k \, d\tau, \tag{13}$$

$$\mathfrak{S}_{ij;k} = \tfrac{1}{2}T\int_S (\delta_{ij} - n_i n_j) x_k \, dS, \tag{14}$$

$$\mathfrak{W}_{ij;k} = \frac{1}{2}\int_V \sigma \mathfrak{W}_{ij} x_k \, d\tau, \tag{15}$$

$$I_{ijk} = \int_V \rho x_i x_j x_k \, d\tau, \tag{16}$$

and

$$\Pi_k = \int_V p x_k \, d\tau. \tag{17}$$

The index following the semicolon in the symbols $\mathfrak{T}_{ij;k}$, $\mathfrak{S}_{ij;k}$, and $\mathfrak{W}_{ij;k}$ indicates that a moment with respect to the associated Cartesian coordinate is involved. The additional factor x_k in the tensors defined by Eqs. (13)–(17), as compared with those defined by Eqs. (6)–(8), (10), and (11), reflects the character of the higher moment. The transformations which lead to the form of Eq. (12) are described in Refs. 13 and 14.

Clearly, virial theorems of higher order can be obtained by taking successively higher moments of the equation of motion. However, in the present considerations we limit our attention to the virial theorems of the first three orders.

The formal development of these tensor virial theorems is independent of the functional forms which the mass and charge distributions may assume. There are no restrictions on the relative internal motions of the fluid. However, no dissipative effects have been included. The formal development of the surface-energy tensors in Ref. 14 has been restricted to closed surfaces on which a *constant* surface tension is operative, but the shape of these surfaces is unrestricted.

These tensor virial theorems provide the basis for an investigation of the equilibrium and the stability of the rotating configurations.

III. EQUILIBRIUM RELATIONS

A. General Considerations

We assume that the equilibrium configurations of the charged liquid drop are initially rotating uniformly with constant angular velocity $\boldsymbol{\Omega}$. These configurations are initially stationary in the chosen frame of reference. The tensor virial theorems must be satisfied when no relative motions are present and a state of hydrostatic equilibrium prevails. Under these conditions, all the velocities and time derivatives in Eqs. (3), (5), and (12) vanish. We obtain

$$0 = \Omega^2(I_i - \delta_{i3} I_3), \tag{18}$$

$$0 = -2\mathfrak{S}_{ij} + \mathfrak{W}_{ij} + \Omega^2(I_{ij} - \delta_{i3} I_{3j}) + \Pi\,\delta_{ij}, \tag{19}$$

and

$$\begin{aligned}0 = &- 2\mathfrak{S}_{ij;k} + \mathfrak{W}_{ij;k} + \delta_{ij}\Pi_k \\ &- 2\mathfrak{S}_{ik;j} + \mathfrak{W}_{ik;j} + \delta_{ik}\Pi_j \\ &+ \Omega^2(I_{ijk} - \delta_{i3} I_{3jk}).\end{aligned} \tag{20}$$

A number of general conclusions follow from these equilibrium relations. It follows from Eq. (18) that

$$I_1 = I_2 = 0, \tag{21}$$

which implies that the axis of rotation must pass through the center of mass. There is no loss of generality in assuming that

$$I_3 = 0 \tag{22}$$

[15] S. Chandrasekhar and N. R. Lebovitz, Astrophys. J. **135**, 238 (1962).
[16] S. Chandrasekhar and N. R. Lebovitz, Astrophys. J. **136**, 1032 (1962).

so that the center of mass is located at the origin. From the components of Eq. (19) for which $i \neq j$, it follows that

$$I_{13} = I_{23} = 0, \tag{23}$$

which implies that the equatorial plane must be a plane of symmetry.[17] However, I_{12} need not vanish so that equilibrium configurations are not necessarily axisymmetric.

The three diagonal components of Eq. (19) may be written in the forms

$$\Omega^2 I_{11} = 2\mathfrak{S}_{11} - \mathfrak{W}_{11} - \Pi, \tag{24}$$

$$\Omega^2 I_{22} = 2\mathfrak{S}_{22} - \mathfrak{W}_{22} - \Pi, \tag{25}$$

and

$$0 = 2\mathfrak{S}_{33} - \mathfrak{W}_{33} - \Pi. \tag{26}$$

Several general inequalities now follow from the physical requirements that both the rotational energy and the quantity Π must be positive for any equilibrium configuration. From the sum of Eqs. (24)–(26), we obtain

$$\Omega^2(I_{11} + I_{22}) = 2\mathfrak{S} - \mathfrak{W} - 3\Pi \geq 0, \tag{27}$$

where $\mathfrak{S}$ is the surface energy and $\mathfrak{W}$ is the potential energy. It follows from expression (27) that

$$\tfrac{2}{3}(\mathfrak{S} - \tfrac{1}{2}\mathfrak{W}) \geq \Pi \geq 0. \tag{28}$$

Finally, from Eq. (26) it follows that

$$\Pi = 2\mathfrak{S}_{33} - \mathfrak{W}_{33} \geq 0. \tag{29}$$

Two very important relations,

$$\Omega^2 I_{11} = 2(\mathfrak{S}_{11} - \mathfrak{S}_{33}) - (\mathfrak{W}_{11} - \mathfrak{W}_{33}) \tag{30}$$

and

$$\Omega^2 I_{22} = 2(\mathfrak{S}_{22} - \mathfrak{S}_{33}) - (\mathfrak{W}_{22} - \mathfrak{W}_{33}), \tag{31}$$

are obtained by using Eq. (26) to eliminate Π from Eqs. (24) and (25). These two relations are used to associate the proper value of Ω^2 with each equilibrium configuration.

The allowed equilibrium configurations are further restricted by the following theorem.

Theorem: Uniformly rotating, axisymmetric, equilibrium configurations cannot have the axis of symmetry perpendicular to the axis of rotation.

Suppose the axis of symmetry lies along x_1. Then it follows quite generally from the definitions of the energy tensors that $\mathfrak{S}_{22} = \mathfrak{S}_{33}$ and $\mathfrak{W}_{22} = \mathfrak{W}_{33}$. Therefore, the right-hand side of Eq. (31) vanishes. Since this conclusion is incompatible with the assumption that $\Omega^2 \neq 0$, the theorem follows. As noted by Beringer and Knox,[8] all of the points, which lie along the intersection of the axisymmetric surface with any plane perpendicular to the axis of symmetry, have the same total curvature and electrostatic potential but are at different distances from the axis of rotation and hence cannot all simultaneously be in equilibrium.

The axis of rotation, on the other hand, may be an axis of symmetry. Under these conditions, Eq. (30) becomes identical with Eq. (31), and the resulting expression determines Ω^2.

We now restrict our attention to configurations which have triplanar symmetry. Under this restriction, all of the off-diagonal components of Eq. (19) vanish identically. In addition, every component of Eq. (20) vanishes identically. Only Eqs. (24)–(26) remain nonvanishing. Therefore, if we can find configurations with triplanar symmetry which satisfy Eqs. (24)–(26), then we have satisfied all of the requirements for equilibrium which follow from the tensor virial theorems through the third order. Under these conditions, we may *assume* that these configurations *are* equilibrium configurations up to at least third order, and we may investigate their stability with respect to second- and third-harmonic deformations.

B. Ellipsoidal and Spheroidal Configurations

Uniformly rotating ellipsoidal configurations which have mass and charge distributions that are initially homogeneous, and which are held together by a constant surface tension, are a particular case of configurations with triplanar symmetry. In order to demonstrate that these configurations can be chosen so as to satisfy Eqs. (24)–(26), we need the expressions for the diagonal components of the energy tensors for homogeneous ellipsoids.

The diagonal components of the surface-energy tensor $\mathfrak{S}_{ij}$ are shown in Ref. 18 to be

$$2\mathfrak{S}_{ii} = 2T(\mathfrak{a}_j + \mathfrak{a}_k) \qquad (i \neq j \neq k), \tag{32}$$

(no summation over repeated i) where the $\mathfrak{a}_i$'s are the one-index symbols for the surface energy. These symbols are defined and evaluated in Ref. 18. In writing T in Eq. (32), we have suppressed the common factor $\pi(a_1 a_2 a_3)^2$. The quantities a_1, a_2, and a_3 are, respectively, the semiaxes of the ellipsoid along x_1, x_2, and x_3.

[17] I. Lichtenstein, *Gleichgewichtsfigüren Rotierender Flüssigkeiten* (Springer-Verlag, Berlin, 1933), p. 12.

[18] C. E. Rosenkilde, J. Math. Phys. 8, 88 (1967).

The diagonal components of the potential-energy tensor $\mathfrak{W}_{ij}$ are shown in Appendix A to be

$$\mathfrak{W}_{ii} = 2\sigma^2 a_i^2 A_i \tag{33}$$

(no summation over repeated i), where the A_i's are the one-index symbols for the potential energy. These symbols were defined and evaluated by Chandrasekhar and Lebovitz.[19] In writing σ^2 in Eq. (33), we have suppressed the common factor $4\pi^2(a_1a_2a_3)^2/15$.

The diagonal components of the moment of inertia tensor are

$$I_{ii} = \rho a_i^2 \tag{34}$$

(no summation over repeated i), where in writing ρ in Eq. (34) we have suppressed the factor

$$4\pi(a_1a_2a_3)/15.$$

In order to satisfy the equilibrium relations (24)–(26), we may choose to *define* Π by Eq. (26). Then, we may proceed with the elimination of

$$\Pi = 2T[\mathcal{A}_1 + \mathcal{A}_2 - (\sigma^2/T)a_3^2 A_3] \tag{35}$$

from Eqs. (24) and (25). The resulting expressions [Eqs. (30) and (31)],

$$(\rho\Omega^2/2T)a_1^2 = \mathcal{A}_3 - \mathcal{A}_1 - (\sigma^2/T)(a_1^2 A_1 - a_3^2 A_3) \tag{36}$$

and

$$(\rho\Omega^2/2T)a_2^2 = \mathcal{A}_3 - \mathcal{A}_2 - (\sigma^2/T)(a_2^2 A_2 - a_3^2 A_3), \tag{37}$$

determine the parameters $\rho\Omega^2/2T$ and σ^2/T for a given ellipsoid with semiaxes a_1, a_2, a_3. When the suppressed constants are restored, we find that σ^2/T represents the fissionability parameter x, and that $\rho\Omega^2/2T$ represents the rotational parameter y, which are used in the theory of nuclear fission. These parameters are explicitly defined in Appendix B.

In this paper we restrict our attention to uniformly rotating spheroids (ellipsoids of revolution) and leave the discussion of triaxial ellipsoids for a subsequent paper.

One can verify, by using the definitions of the multi-index symbols in the case that $a_2 = a_3$, that neither prolate nor oblate spheroids can satisfy Eq. (37) when $\Omega^2 \neq 0$, in agreement with the above theorem. (It should be noted that this theorem does not apply to cases considered by Bohr.[20] Those configurations do not rotate uniformly, and internal motions are present.) Since the equatorial plane of any equilibrium configuration must be a plane of symmetry, the spheroids must rotate about their axis of symmetry. Under these conditions, Eq. (36) and (37) are identical ($a_1 = a_2$). By using the identities satisfied by the multi-index symbols, we can rewrite Eq. (36) in the form

$$\frac{\rho\Omega^2}{2T} = \left(1 - \frac{a_3^2}{a_1^2}\right)\left(\mathcal{A}_{13} - \frac{\sigma^2}{T}B_{13}\right). \tag{38}$$

(Beringer and Knox[8] obtained an equivalent relation from an energy principle by using a shape-preserving deformation.)

The allowed equilibrium configurations are further restricted by the inequality (29), which takes the form

$$\Pi = 2T[2\mathcal{A}_1 - (\sigma^2/T)a_3^2 A_3] \geq 0. \tag{39}$$

Therefore, the amount of charge in a given spheroid is limited by the relation

$$\sigma^2/T \leq 2\mathcal{A}_1/a_3^2 A_3. \tag{40}$$

(In the limit of no rotation, this relation reduces to the requirement that a spherical drop must have $x \leq 1$; see Appendix E.)

The equilibrium configurations defined by Eqs. (38) and (40) are of two types. There are sequences of oblate spheroids which we identify later as rotating ground-state configurations. There are also sequences of prolate spheroids, rotating about the axis of symmetry, which we later identify as first approximations to a particular class of rotating saddle-shape configurations. In Sec. VII we discuss each of these types of configurations and indicate to what extent these shapes approximate the exact axisymmetric figures of equilibrium for a rotating charged liquid drop.

IV. VIRIAL EQUATIONS FOR SMALL OSCILLATIONS ABOUT EQUILIBRIUM

We assume that a uniformly rotating charged liquid drop, initially in a state of equilibrium, is slightly perturbed; and further that the ensuing motions are described by a Lagrangian displacement of the form

$$\xi(\mathbf{x})e^{\lambda t}, \tag{41}$$

where λ is a parameter whose characteristic values are to be determined. To first order in ξ, the first variations of the tensor virial theorems of the first, second, and third orders give

$$\lambda^2 V_i - 2\lambda\Omega\epsilon_{i13}V_l = \Omega^2(\delta I_i - \delta_{i3}\,\delta I_3), \tag{42}$$

[19] S. Chandrasekhar and N. R. Lebovitz, Astrophys. J. **136**, 1037 (1962).

[20] A. Bohr, *Rotational States of Atomic Nuclei* (Ejnar Munksgaards Forlag, Copenhagen, 1954).

$$\lambda^2 V_{i;j} - 2\lambda\Omega\epsilon_{i\ell 3}V_{\ell;j} = -2\delta\mathfrak{S}_{ij} + \delta\mathfrak{W}_{ij} + \Omega^2(\delta I_{ij} - \delta_{i3}\,\delta I_{3j}) + \delta\Pi\,\delta_{ij}, \tag{43}$$

and

$$\lambda^2 V_{i;jk} - 2\lambda\Omega\epsilon_{i\ell 3}V_{\ell;jk} = -2\delta\mathfrak{S}_{ij;k} + \delta\mathfrak{W}_{ij;k} + \delta_{ij}\,\delta\Pi_k - 2\delta\mathfrak{S}_{ik;j} + \delta\mathfrak{W}_{ik;j} + \delta_{ik}\,\delta\Pi_j + \Omega^2(\delta I_{ijk} - \delta_{i3}\,\delta I_{3jk}), \tag{44}$$

where

$$V_i = \int_V \rho\xi_i\, d\tau, \tag{45}$$

$$V_{i;j} = \int_V \rho\xi_i x_j\, d\tau, \tag{46}$$

and

$$V_{i;jk} = \int_V \rho\xi_i x_j x_k\, d\tau. \tag{47}$$

In deriving Eqs. (42)–(44) from Eqs. (3), (5), and (12), the first variation of Ω vanishes, since it represents the constant angular velocity of the rotating frame of reference. Although Ω has been chosen so that the undisturbed equilibrium configuration is initially stationary in this frame of reference, after the perturbation the disturbed configuration is, in general, no longer stationary in this frame. It is, nevertheless, moving in such a way that its total angular momentum (as referred in a *nonrotating* frame) is still conserved. This is a general consequence of the time-dependent character of the tensor virial theorems.

The virials of the first order V_i are equal to the variations in the position of the center of mass

$$\delta I_i = V_i. \tag{48}$$

Equation (42) is a kinematic relation; it is independent of any energy tensors, and hence it is independent of the construction and the constitution of the system under investigation. Therefore, in the subsequent discussion, there is no loss of generality in assuming that

$$V_i = 0. \tag{49}$$

This means that the perturbed motion will be viewed from a uniformly translating frame of reference in which the center of mass is permanently located at the origin. (This is equivalent to the center-of-mass correction made by Present and Knipp.[21])

[21] R. D. Present and J. K. Knipp, Phys. Rev. 57, 751 (1940).

The unsymmetrized virials of the second order $V_{i;j}$ are related to the variations in the moment of inertia tensor:

$$\delta I_{ij} = V_{i;j} + V_{j;i} = V_{ij}, \tag{50}$$

where the V_{ij}'s (without the semicolon) are the symmetrized virials of the second order. The unsymmetrized virials of the third order $V_{i;jk}$ are related to the variations in the third moments of the mass distribution:

$$\delta I_{ijk} = V_{i;jk} + V_{j;ki} + V_{k;ij} = V_{ijk}, \tag{51}$$

where the V_{ijk}'s are the symmetrized virials of the third order.

Clearly, the variations of higher-order virial theorems require the introduction of higher-order virials. However, the present considerations are limited to the virial theorems of orders one, two, and three. The space dependence of the Lagrangian displacement cannot involve any more unknown parameters than the total number of virial equations to be considered (a total of 30 in this case.) Under these conditions, an appropriate choice for the form of $\xi(\mathbf{x})$ is

$$\xi_i = L_i + \sum_j L_{i;j}x_j + \sum_{j,k} L_{i;jk}x_j x_k, \tag{52}$$

where the L's are undetermined constants. [Further discussion regarding this choice for ξ is given in Appendix D of Ref. 18.] Since i may assume the values 1 to 3, there are a total of three L_i's, nine $L_{i;j}$'s, and eighteen $L_{i;jk}$'s ($L_{i;jk} = L_{i;ki}$, by symmetry). The 30 virials V_i, $V_{i;j}$, and $V_{i;jk}$ are linear functions of these undetermined constants [cf., Ref. 18, Eqs. (55) and (77)–(81)]. In view of this linear relationship, there is no loss of generality in retaining the virials themselves as the parameters to be determined by the virial equations.

We need expressions for the variations $\delta\mathfrak{S}_{ij}$, $\delta\mathfrak{S}_{ij;k}$, $\delta\mathfrak{W}_{ij}$, and $\delta\mathfrak{W}_{ij;k}$. The specification of these variations in terms of ξ has been given in Ref. 14. Expressions for $\delta\mathfrak{S}_{ij}$ and $\delta\mathfrak{S}_{ij;k}$ in terms of the virials have been given in Ref. 18. The expressions for $\delta\mathfrak{W}_{ij}$ and $\delta\mathfrak{W}_{ij;k}$ in terms of the virials can be obtained from Refs. 13 and 22, when account is taken of the sign conventions discussed in Appendix A.

The specification of $\delta\Pi$ and $\delta\Pi_k$ in terms of ξ requires some supplementary assumption concerning the physical nature of the oscillations. For an incompressible fluid, the Lagrangian displacement is

[22] S. Chandrasekhar and N. R. Lebovitz, Astrophys. J. 137, 1142 (1963).

required to be solenoidal in order to preserve the total volume. The restriction

$$\operatorname{div} \xi = 0, \tag{53}$$

imposes four additional relations among the virials of the first three orders. For ellipsoids, we have

$$\sum_{i=1}^{3} \frac{V_{ii}}{a_i^2} = 0 \tag{54}$$

and, by making use of Eq. (49),

$$\sum_{i=1}^{3} \frac{V_{iii}}{a_i^2} = V_i = 0, \qquad i = 1, 2, 3. \tag{55}$$

If we supplement the set of virial equations with these four relations, then we may dispense with the evaluation of $\delta\Pi$ and $\delta\Pi_k$ ($k = 1, 2, 3$) and eliminate them from the system.

Since the virial equations of even order are independent of those of odd order, we may discuss the symmetric and asymmetric deformations separately.

V. OSCILLATIONS BELONGING TO THE SECOND HARMONICS

We use the virial equations of the second order to investigate the stability of the axisymmetric equilibrium configurations with respect to second-harmonic deformations. The conditions for the onset of instability follow from an examination of the nature of the characteristic frequencies of oscillation belonging to these symmetric deformations.

The nine virial equations, which follow from Eq. (43), separate into two noncombining groups distinguished by their parity (i.e., evenness or oddness) with respect to the index 3. There are five equations of even parity and four equations of odd parity. The analysis of these equations closely resembles the corresponding analyses given by Chandrasekhar for the self-gravitating Maclaurin spheroid[13] and for the uncharged liquid drop.[23] The correspondence is complete if, for example, the quantity $\delta\mathfrak{W}_{ij}$ in Chap. VI of Ref. 13 is replaced by the combination

$$-\delta\mathfrak{U}_{ij} = -2\delta\mathfrak{S}_{ij} + \delta\mathfrak{W}_{ij}. \tag{56}$$

By taking appropriate linear combinations of the five equations of even parity (in the present case of axisymmetry), two noncombining groups can be formed. The first group (hereafter called Group A) contains the two equations

$$\lambda^2 V_{12} + 2\lambda\Omega(V_{1;1} - V_{2;2}) = -2\delta\mathfrak{U}_{12} + 2\Omega^2 V_{12} = 2(\Omega^2 - P)V_{12} \tag{57}$$

and

$$\lambda^2(V_{1;1} - V_{2;2}) - 2\lambda\Omega V_{12} = -(\delta\mathfrak{U}_{11} - \delta\mathfrak{U}_{22}) + \Omega^2(V_{11} - V_{22}) = 2(\Omega^2 - P)(V_{1;1} - V_{2;2}), \tag{58}$$

where

$$P = (2T/\rho)[\mathfrak{A}_{11} - (\sigma^2/T)B_{11}]. \tag{59}$$

The quantity P in Eqs. (57) and (58) is obtained by combining the appropriate components of Eqs. (A4) and (A5) in Appendix A with Eqs. (66) and (69) of Ref. 18.

The remaining equations of even parity involve $\delta\Pi$. If we use the 3, 3-component of Eq. (43) to eliminate $\delta\Pi$ from the system and supplement the remaining equations with the divergence condition (54), then we find that the second group (hereafter called Group B) contains the three equations

$$\lambda^2(V_{1;2} - V_{2;1}) - 2\lambda\Omega(V_{1;1} + V_{2;2}) = 0, \tag{60}$$

$$\lambda^2(V_{1;1} + V_{2;2} - 2V_{3;3}) + 2\lambda\Omega(V_{1;2} - V_{2;1}) = -(\delta\mathfrak{U}_{11} + \delta\mathfrak{U}_{22} - 2\delta\mathfrak{U}_{33}) + \Omega^2(V_{11} + V_{22}) = 2(\Omega^2 - M)(V_{1;1} + V_{2;2}) + 2NV_{3;3}, \tag{61}$$

and

$$a_1^{-2}(V_{1;1} + V_{2;2}) + a_3^{-2}V_{3;3} = 0, \tag{62}$$

where

$$M = \frac{2T}{\rho}\left[2\mathfrak{A}_{11} - \frac{a_3^2}{a_1^2}\mathfrak{A}_{13} - \frac{\sigma^2}{T}(2B_{11} - B_{13})\right] \tag{63}$$

and

$$N = \frac{2T}{\rho}\left[3\mathfrak{A}_{33} - \frac{a_1^2}{a_3^2}\mathfrak{A}_{13} - \frac{\sigma^2}{T}(3B_{33} - B_{13})\right]. \tag{64}$$

In obtaining the expressions for M and N, we have made use of Eqs. (70) and (71) in Ref. 18, Eq. (A5) in Appendix A, and the recursion relations satisfied by each type of multi-index symbol.

The four equations of odd parity (hereafter called Group C) are

$$\lambda^2 V_{1;3} - 2\lambda\Omega V_{2;3} = -\delta\mathfrak{U}_{13} + \Omega^2 V_{13} = (\Omega^2 - Q)V_{13}, \tag{65}$$

$$\lambda^2 V_{2;3} + 2\lambda\Omega V_{1;3} = -\delta\mathfrak{U}_{23} + \Omega^2 V_{23} = (\Omega^2 - Q)V_{23}, \tag{66}$$

$$\lambda^2 V_{3;1} = -\delta\mathfrak{U}_{31} = -QV_{31}, \tag{67}$$

and

$$\lambda^2 V_{3;2} = -\delta\mathfrak{U}_{32} = -QV_{32}, \tag{68}$$

[23] S. Chandrasekhar, Proc. Roy. Soc. (London) **A286**, 1 (1964).

where

$$Q = (2T/\rho)[\mathfrak{A}_{13} - (\sigma^2/T)B_{13}]. \tag{69}$$

The quantity Q is obtained by combining the appropriate components of Eq. (A4) in Appendix A with Eqs. (67) and (68) of Ref. 18.

The virial equations which describe the oscillations of the Maclaurin spheroid and the uncharged liquid drop separate into exactly these same three symmetry groups. In the context of gravitation, the natural modes of oscillation associated with the Groups A, B, and C are known, respectively, as the toroidal modes, the pulsation modes, and the transverse-shear modes. In nuclear physics, the toroidal and pulsation modes are known as the γ and β vibrations, respectively. We treat the toroidal modes first since it is by these modes that the rotating charged liquid drop manifests both neutral stability and overstability.

A. Toridal Modes (γ Vibration)

Group A depends only upon $V_{1;1} - V_{2;2}$ and V_{12}. It follows that the appropriate displacement for these modes is

$$\xi_1 = L_{1;1}x_1 + L_{1;2}x_2, \qquad \xi_2 = L_{1;2}x_1 - L_{1;1}x_2, \quad \text{and} \quad \xi_3 = 0. \tag{70}$$

This displacement transforms a given spheroid into a triaxial ellipsoid; it corresponds to the γ vibration.

The characteristic equation for these modes is

$$(\lambda^2 + 2P - 2\Omega^2)^2 + 4\lambda^2\Omega^2 = 0. \tag{71}$$

If we replace λ^2 by $-\omega^2$ (so that a real ω is a necessary and sufficient condition for the stability of these modes), then Eq. (71) can be written in two equivalent forms:

$$\omega^4 - 4\omega^2 P + 4(\Omega^2 - P)^2 = 0 \tag{72}$$

or

$$[(\omega + \Omega)^2 + \Omega^2 - 2P] \times [(\omega - \Omega)^2 + \Omega^2 - 2P] = 0. \tag{73}$$

From Eq. (72), it follows that a neutral mode ($\omega = 0$) of multiplicity 2 obtains when

$$\Omega^2 = P = (2T/\rho)[\mathfrak{A}_{11} - (\sigma^2/T)B_{11}]. \tag{74}$$

At this neutral point the perturbation has no sinusoidal time dependence. Moreover, when $\omega^2 = 0$, Eqs. (57) and (58) do not allow any perturbation which has a linear time dependence. Therefore, this neutral point indicates the occurrence of a point of bifurcation along a sequence of axisymmetric equilibrium configurations.

At this point of bifurcation, genuine tri-axial configurations (in this case, ellipsoids) first become possible figures of equilibrium. The values of x and y associated with this point of bifurcation are given by the simultaneous solution of Eqs. (38) and (74):

$$\frac{\sigma^2}{T} = \frac{a_1^2\mathfrak{A}_{11} - (a_1^2 - a_3^2)\mathfrak{A}_{13}}{a_1^2 B_{11} - (a_1^2 - a_3^2)B_{13}}, \tag{75}$$

$$\frac{\rho\Omega^2}{2T} = \frac{(a_1^2 - a_3^2)(\mathfrak{A}_{13}B_{11} - \mathfrak{A}_{11}B_{13})}{a_1^2 B_{11} - (a_1^2 - a_3^2)B_{13}}. \tag{76}$$

In Appendix C, we verify that a sequence of rotating ellipsoids branches off from a sequence of rotating spheroids at these values of x and y.

The form of Eq. (72) implies that ω^2 does not change sign when the quantity $\Omega^2 - P$ changes sign. Therefore, in the absence of any dissipative mechanism,[24] *no instability occurs at this point of bifurcation.*

The four characteristic roots of Eq. (73) are

$$\omega = \pm[\Omega \pm (2P - \Omega^2)^{\frac{1}{2}}]. \tag{77}$$

These frequencies of oscillation cease to be real when

$$\Omega^2 = 2P. \tag{78}$$

For greater values of Ω^2, the axisymmetric configurations admit overstable oscillations (complex ω), and are, therefore, unstable. The values of x and y associated with this overstable point are given by the simultaneous solution of Eqs. (38) and (78):

$$\frac{\sigma^2}{T} = \frac{2a_1^2\mathfrak{A}_{11} - (a_1^2 - a_3^2)\mathfrak{A}_{13}}{2a_1^2 B_{11} - (a_1^2 - a_3^2)B_{13}}, \tag{79}$$

$$\frac{\rho\Omega^2}{2T} = \frac{2(a_1^2 - a_3^2)(\mathfrak{A}_{13}B_{11} - \mathfrak{A}_{11}B_{13})}{2a_1^2 B_{11} - (a_1^2 - a_3^2)B_{13}}. \tag{80}$$

We defer until Sec. VII the quantitative discussion of the values of x and y associated with these points of bifurcation and overstability along the sequences of spheroids. However, one qualitative conclusion concerning the *exact* axisymmetric configurations can be inferred at this point. The separation of Group A from the rest of the equations of even parity depends only upon the axisymmetry of the configurations and is independent of the divergence condition. Therefore these equations are relatively insensitive to the particular properties

[24] P. H. Roberts and K. Stewartson, Astrophys. J. 137, 777 (1963), have shown that the viscous Maclaurin spheroids become unstable at the point of bifurcation.

of a shape which already possesses the proper symmetry. This implies that the exact axisymmetric configurations also exhibit the above points of bifurcation and overstability in exactly the same manner. This appears as a general property of uniformly rotating, axisymmetric, homogeneous fluid configurations without dissipation.

B. Pulsation Modes (β Vibration)

Group B depends only upon $V_{1;2}-V_{2;1}$, $V_{1;1}+V_{2;2}$, and $V_{3;3}$. It follows that the appropriate displacement for these modes is

$$\xi_1 = L_{1;1}x_1 + L_{1;2}x_2, \qquad \xi_2 = -L_{1;2}x_1 + L_{1;1}x_2, \quad \text{and} \quad \xi_3 = -2L_{1;1}x_3. \tag{81}$$

This displacement preserves the axisymmetry and transforms a given spheroid into a neighboring spheroid having a slightly different eccentricity; it corresponds to the β vibration.

The characteristic equation for these modes is

$$\lambda^2\{\lambda^2[1 + (2a_3^2/a_1^2)] + 2[\Omega^2 + M + (a_3^2/a_1^2)N]\} = 0. \tag{82}$$

If we replace λ^2 by $-\omega^2$ (a real ω implies stability), then in addition to the pair of zero roots, Eq. (82) allows the roots

$$\omega = \pm\sqrt{2}\,[1 + (2a_3^2/a_1^2)]^{-\frac{1}{2}} \times [\Omega^2 + M + (a_3^2/a_1^2)N]^{\frac{1}{2}}. \tag{83}$$

These roots are real in the case of oblate spheroids and imaginary in the case of prolate spheroids.

The two zero roots do not indicate the occurrence of a point of bifurcation (cf., Lebovitz[25]). However, they do indicate the presence of two nonoscillatory solutions of Eqs. (60)–(62). One of these solutions for which $V_{1;1} + V_{2;2} = 0$ and $V_{1;2} - V_{2;1}$ is an arbitrary constant, corresponds to an infinitesimal rotation of the spheroid about x_3 without any change of shape. The other solution has a linear time dependence of the form $V_{1;1} + V_{2;2} = b$ and

$$V_{1;2} - V_{2;1} = a - (b/\Omega)[M + (a_3^2/a_1^2)N - \Omega^2]t, \tag{84}$$

where a and b are arbitrary constants. It corresponds to the infinitesimal displacement which generates the sequence of rotating axisymmetric equilibrium configurations starting from the sphere. The equilibrium is preserved by changing the rate of rotation from Ω to $\Omega + \delta\Omega$ and by simultaneously altering the shape of the spheroid from that appropriate to Ω to that appropriate to $\Omega + \delta\Omega$. (The magnitude but not the direction of the angular momentum is changed during this displacement.) If Ω should pass through an extremum value along the sequence, then $\delta\Omega$ must vanish, and in the frame of reference with this value of Ω, there should not be any time dependence in Eq. (84). By starting from Eq. (38), one can indeed verify that the condition $\delta\Omega = 0$ is satisfied when

$$\Omega^2 = M + (a_3^2/a_1^2)N. \tag{85}$$

A similar phenomenon occurs along the sequence of Maclaurin spheroids.[13]

C. Transverse-Shear Modes

Group C depends only upon $V_{1;3}$, $V_{2;3}$, $V_{3;1}$, and $V_{3;2}$. It follows that the appropriate displacement for these modes is

$$\xi_1 = L_{1;3}x_3, \qquad \xi_2 = L_{2;3}x_3, \quad \text{and} \quad \xi_3 = L_{3;1}x_1 + L_{3;2}x_2. \tag{86}$$

This displacement induces relative motion of the two hemispheres; the spheroid tilts over and simultaneously may become an ellipsoid.

The characteristic equation for these modes is

$$\lambda^2[\lambda^2(\lambda^2 - \Omega^2 + 2Q)^2 + 4\Omega^2(\lambda^2 + Q)^2] = 0. \tag{87}$$

If we replace λ^2 by $-\omega^2$ (a real ω implies stability), then Eq. (87) can be factored in the form

$$\omega^2[(\omega - \Omega)(\omega^2 - \omega\Omega - 2Q)] \times [(\omega + \Omega)(\omega^2 + \omega\Omega - 2Q)] = 0. \tag{88}$$

It follows that the eight characteristic roots are

$$\omega = \pm\tfrac{1}{2}[\Omega \pm (\Omega^2 + 8Q)^{\frac{1}{2}}], \tag{89}$$

$\omega = \pm\Omega$, and $\omega = 0$ (of multiplicity 2).

By using the equilibrium equation (38), which can be written as

$$\Omega^2 = (1 - a_3^2/a_1^2)Q, \tag{90}$$

we can rewrite Eq. (89) in the form

$$\omega = \pm\tfrac{1}{2}\Omega\{1 \pm [(9a_1^2 - a_3^2)/(a_1^2 - a_3^2)]^{\frac{1}{2}}\}. \tag{91}$$

It follows that oblate spheroids ($a_3 < a_1$) are completely stable with respect to the transverse-shear modes. However, prolate spheroids ($a_3 > a_1$) are stable with respect to these modes only when $a_3 \geq 3a_1$. The prolate spheroids are overstable when $a_1 < a_3 < 3a_1$.

The displacement associated with the roots $\pm\Omega$ corresponds to an infinitesimal rotation of the spheroid about x_1 or x_2 without any change of

[25] N. R. Lebovitz, Astrophys. J. 138, 1214 (1963).

shape. The direction of the angular momentum is changed during this displacement. The pair of zero roots belong to the proper solution for which both V_{13} and V_{23} vanish. The associated displacement leaves the spheroid upright but induces infinitesimal internal motions having a uniform vorticity along x_1 or x_2.

We have obtained a total of six nonvanishing values of ω^2 in the second order in agreement with a lemma of Cartan.[26]

VI. OSCILLATIONS BELONGING TO THE THIRD HARMONICS

We use the virial equations of the third order to investigate the stability of the axisymmetric equilibrium configurations with respect to third-harmonic deformations. The possible occurrence of additional points of bifurcation is of particular interest. The limits of stability with respect to these asymmetric deformations can be obtained from the characteristic equations for the frequencies of oscillation.

The 18 virial equations, which follow from Eq. (44), separate into two noncombining groups distinguished by their parity with respect to the index 3. There are 10 equations of even parity and 8 equations of odd parity. In analyzing these equations, we are guided, initially, by the corresponding investigations of the third-harmonic oscillations of the Jacobi ellipsoids and of the Maclaurin spheroids, which have been given by Chandrasekhar and Lebovitz.[22,27]

The virial equations of the third order, which are appropriate for a rotating charged liquid drop, may be obtained explicitly from Eqs. (26)–(43) of Ref. 22 by replacing the components of $-\delta\mathfrak{W}_{ij;k}$ in each of those equations by the corresponding components of

$$\delta\mathfrak{U}_{ij;k} = 2\delta\mathfrak{S}_{ij;k} - \delta\mathfrak{W}_{ij;k}. \tag{92}$$

Later the quantity $\delta\mathfrak{S}_{ij;j}$ [Ref. 22, Eq. (62)] may be replaced by the quantity

$$\delta\mathfrak{U}_{ij;j} = 4\delta\mathfrak{U}_{ij;j} + 2\delta\mathfrak{U}_{jj;i} - 2\delta\mathfrak{U}_{ii;i} \tag{93}$$

(no summation over repeated indices). Expressions for $\delta\mathfrak{S}_{ij;k}$ for homogeneous spheroids are given in Table II of Ref. 18. The correct expressions for $\delta\mathfrak{W}_{ij;k}$ for homogeneous spheroids may be obtained from Table I of Ref. 22 or Table I of Ref. 27 when account is taken of the sign conventions discussed in Appendix A.

A. Equations of Even Parity

The 10 equations of even parity correspond to Eqs. (26)–(35) of Ref. 22. These equations can be rearranged into a form corresponding to Eqs. (48)–(57) of Ref. 22. In this latter form, the quantities $\delta\Pi_1$ and $\delta\Pi_2$ can be eliminated. The resulting eight equations, which correspond to Eqs. (58)–(61) and (64)–(67) of Ref. 22, separate into two groups.

The two equations (hereafter called Group D) which correspond to Eqs. (58) and (59) of Ref. 22 contain, respectively, the quantities $\delta\mathfrak{U}_{122}$ and $\delta\mathfrak{U}_{211}$. According to the tables, the expansions for these quantities contain no terms in V_{133} and V_{233}; and, moreover,

$$\delta\mathfrak{U}_{122} = P_1(V_{122} - \tfrac{1}{3}V_{111}) \tag{94}$$

and

$$\delta\mathfrak{U}_{211} = P_1(V_{211} - \tfrac{1}{3}V_{222}), \tag{95}$$

where

$$P_1 = (3T'/\rho)[7(\mathfrak{A}_{11} - 2\mathfrak{B}_{111}) - (2\sigma^2/T)(B_{11} + a_1^2 B_{111})]. \tag{96}$$

Therefore, Group D takes the form [cf., Eqs. (2) and (3) of Ref. 27]

$$(\lambda^2 - 3\Omega^2 + P_1)(V_{122} - \tfrac{1}{3}V_{111}) + 2\lambda\Omega(V_{211} - \tfrac{1}{3}V_{222}) = 0, \tag{97}$$

$$(\lambda^2 - 3\Omega^2 + P_1)(V_{211} - \tfrac{1}{3}V_{222}) - 2\lambda\Omega(V_{122} - \tfrac{1}{3}V_{111}) = 0. \tag{98}$$

The remaining six equations (hereafter called Group E) correspond to Eqs. (60), (61), and (64)–(67) of Ref. 22. It is convenient to rearrange these equations and make explicit use of the divergence conditions

$$a_1^{-2}(V_{111} + V_{122}) + a_3^{-2}V_{133} = 0 \tag{99}$$

and

$$a_1^{-2}(V_{222} + V_{211}) + a_3^{-2}V_{233} = 0 \tag{100}$$

at this point. We have the group (see Appendix D)

$$[\lambda^2(4 + \alpha) + (4 + 11\alpha)(M_1 - \Omega^2) + \alpha N_1]V_{133} + 8\lambda\Omega(V_{2;11} - V_{2;33}) = (3\Omega^2 - P_1 - \lambda^2)(V_{122} - \tfrac{1}{3}V_{111}), \tag{101}$$

[26] E. Cartan, in *Proceedings of the International Mathematical Conference, 1924*, J. C. Fields, Ed. (University of Toronto Press, Toronto, Canada, 1928), Vol. 2, p. 9.

[27] S. Chandrasekhar and N. R. Lebovitz, Astrophys. J. 137, 1162 (1963).

$$[\lambda^2(4+\alpha)+(4+11\alpha)(M_1-\Omega^2)+\alpha N_1]V_{233} - 8\lambda\Omega(V_{1;22}-V_{1;33}) = (3\Omega^2-P_1-\lambda^2)(V_{211}-\tfrac{1}{3}V_{222}), \quad (102)$$

$$\lambda^2 V_{1;33}-2\lambda\Omega V_{2;33}+(M_1-\Omega^2)V_{133}=0, \quad (103)$$

$$\lambda^2 V_{2;33}+2\lambda\Omega V_{1;33}+(M_1-\Omega^2)V_{233}=0, \quad (104)$$

$$4\lambda^2 V_{1;22}+2\alpha\lambda\Omega V_{233}-\alpha(M_1-\Omega^2)V_{133} = (3\Omega^2-P_1)(V_{122}-\tfrac{1}{3}V_{111}) - 2\lambda\Omega(V_{211}-\tfrac{1}{3}V_{222}), \quad (105)$$

$$4\lambda^2 V_{2;11}-2\alpha\lambda\Omega V_{133}-\alpha(M_1-\Omega^2)V_{233} = (3\Omega^2-P_1)(V_{211}-\tfrac{1}{3}V_{222}) + 2\lambda\Omega(V_{122}-\tfrac{1}{3}V_{111}), \quad (106)$$

where

$$M_1=(5T/\rho)[7\mathfrak{B}_{113}-(\sigma^2/T)(B_{13}-a_1^2B_{113})], \quad (107)$$

$$N_1=(30T/\rho)(1-a_3^2/a_1^2)(\mathfrak{A}_{13}-7\mathfrak{B}_{113}), \quad (108)$$

and

$$\alpha=a_1^2/a_3^2. \quad (109)$$

1. Group D

This group depends only upon the quantities $V_{122}-\frac{1}{3}V_{111}$ and $V_{211}-\frac{1}{3}V_{222}$. The characteristic equation is

$$(\lambda^2-3\Omega^2+P_1)^2+4\lambda^2\Omega^2=0. \quad (110)$$

If we replace λ^2 by $-\omega^2$ (a real ω implies stability), then Eq. (110) can be written in two equivalent forms:

$$\omega^4+2\omega^2(\Omega^2-P_1)+(3\Omega^2-P_1)^2=0 \quad (111)$$

or

$$[(\omega+\Omega)^2+2\Omega^2-P_1] \times [(\omega-\Omega)^2+2\Omega^2-P_1]=0. \quad (112)$$

From Eq. (111), it follows that a neutral mode ($\omega=0$) of multiplicity 2 obtains when

$$3\Omega^2=P_1. \quad (113)$$

At this neutral point the perturbation has no sinusoidal time dependence. Moreover, when $\omega^2=0$, Eqs. (97) and (98) do not allow any perturbation which has a linear time dependence. Therefore, this neutral point indicates the occurrence of an addition point of bifurcation along a sequence of axisymmetric equilibrium configurations.

At this point of bifurcation, genuine asymmetric configurations first become possible figures of equilibrium. The values of x and y associated with this point of bifurcation are given by the simultaneous solution of Eqs. (38) and (113):

$$\frac{\sigma^2}{T}=\frac{7a_1^2(\mathfrak{A}_{11}-2\mathfrak{B}_{111})-2(a_1^2-a_3^2)\mathfrak{A}_{13}}{2a_1^2(B_{11}+a_1^2B_{111})-2(a_1^2-a_3^2)B_{13}}, \quad (114)$$

$$\frac{\rho\Omega^2}{2T}=(a_1^2-a_3^2) \times\left[\frac{2\mathfrak{A}_{13}(B_{11}+a_1^2B_{111})-7(\mathfrak{A}_{11}-2\mathfrak{B}_{111})B_{13}}{2a_1^2(B_{11}+a_1^2B_{111})-2(a_1^2-a_3^2)B_{13}}\right]. \quad (115)$$

The form of Eq. (111) implies that ω^2 does not change sign when the quantity $3\Omega^2-P_1$ changes sign. Therefore, in the absence of any dissipative mechanism, no instability occurs at this point of bifurcation.

The four characteristic roots of Eq. (112) are

$$\omega=\pm[\Omega\pm(P_1-2\Omega^2)^{\frac{1}{2}}]. \quad (116)$$

These frequencies of oscillation cease to be real when

$$\Omega^2=2P_1. \quad (117)$$

For greater values of Ω^2, the configurations admit overstable oscillations (complex ω), and are, therefore, unstable. The values of x and y associated with this overstable point are given by the simultaneous solution of Eqs. (38) and (117), which is similar to Eqs. (114) and (115).

In order to illuminate the nature of the asymmetric figures of equilibrium, it is of interest to obtain the Lagrangian displacement which generates these figures at the point of bifurcation. The appropriate displacement must not affect the equations of odd parity. Therefore, all of the virials which are odd in the index 3 must vanish. In view of the equality of a_1 and a_2, there is no loss of generality in supposing that all of the virials which are odd in the index 2 also vanish. Group D is independent of the quantity V_{133} so that we may choose

$$V_{133}=0. \quad (118)$$

At the point of bifurcation [where $\lambda=0$ and Eq. (113) is satisfied] the coupling between Groups D and E is broken so that the displacement we seek must be orthogonal to any displacement that is appropriate for Group E. Finally, the displacement must still allow

$$V_{122}-\tfrac{1}{3}V_{111}=\tfrac{4}{3}V_{122}\neq 0. \quad (119)$$

The only displacement which satisfies all of these requirements is the displacement

$$\xi_i=\tfrac{1}{3}c(\partial/\partial x_i)(x_1^3-3x_1x_2^2), \quad (120)$$

whose components are

$$\xi_1 = c(x_1^2 - x_2^2), \qquad \xi_2 = -2cx_1x_2, \quad \text{and} \quad \xi_3 = 0, \tag{121}$$

where c is an arbitrary infinitesimal constant. This displacement generates a figure of equilibrium which has three identical lobes symmetrically placed around the axis of rotation.

The phenomena of bifurcation and overstability exhibited here by a rotating charged liquid drop also occurs in exactly the same manner for the Maclaurin spheroids.[27] In that case, Chandrasekhar[28] obtained the point of bifurcation in a slightly different (although equivalent) way.

2. Group E

In analyzing Group E, we must require

$$V_{122} - \tfrac{1}{3}V_{111} = V_{211} - \tfrac{1}{3}V_{222} = 0, \tag{122}$$

so that we may not be inconsistent with the equations in Group D. Because of this requirement the terms on the right-hand sides of Eqs. (101), (102), (105), and (106) vanish. Group E then depends only upon $V_{1;33}$, $V_{2;33}$, $V_{2;11}$, $V_{1;22}$, V_{133}, and V_{233}.

The characteristic equation for these modes is

$$\lambda^4\{(\lambda^2 + 4\Omega^2)[\lambda^2(\beta\lambda^2 + r)^2 + 4\Omega^2\alpha^2s^2] - 32\lambda^2\Omega^2s[\beta\lambda^2 + r - (2 + \alpha)s]\} = 0, \tag{123}$$

where

$$r = (4 + 11\alpha)s + \alpha(4\Omega^2 + N_1), \tag{124}$$

$$s = M_1 - \Omega^2, \tag{125}$$

and

$$\beta = 4 + \alpha. \tag{126}$$

In addition to the factor λ^4, Eq. (123) contains a polynomial of degree four in λ^2. If we replace λ^2 by $-\omega^2$, then this polynomial can be written as the product of two quartic factors. We have

$$\beta\omega^4 \pm 2\beta\Omega\omega^3 - r\omega^2 \mp 2\Omega(r - \beta s)\omega + 4\alpha\Omega^2 s = 0. \tag{127}$$

It follows from Eq. (127) that a neutral mode ($\omega = 0$) obtains when

$$s = M_1 - \Omega^2 = 0. \tag{128}$$

However, we shall verify that this neutral mode does *not* indicate the occurrence of a point of bifurcation along the sequence of axisymmetric equilibrium configurations for the rotating charged liquid drop.

[28] S. Chandrasekhar, Astrophys. J. 137, 1185 (1963).

This neutral point can be a point of bifurcation if Eqs. (101)–(106) admit only time-independent perturbations when $\lambda = 0$ (i.e., the perturbation should not have any polynomial time dependence). These requirements can be achieved only if the pair of equations

$$[(4 + 11\alpha)(M_1 - \Omega^2) + \alpha N_1]V_{133} = 0, \tag{129}$$

$$(M_1 - \Omega^2)V_{133} = 0, \tag{130}$$

and a similar pair which involves V_{233}, can be simultaneously satisfied with nonvanishing virials. This is possible only when N_1 vanishes and Eq. (128) is satisfied. However, N_1 is proportional to the nonvanishing factor

$$\mathfrak{A}_{13} - 7\mathfrak{B}_{113} = 3(\mathfrak{B}_{133} - \mathfrak{B}_{113}) = 3(a_1^2 - a_3^2)\mathfrak{B}_{1133} \neq 0, \tag{131}$$

where $\mathfrak{B}_{1133}$ is a four-index symbol in the notation used in Ref. 18. Therefore, N_1 does not vanish, and this neutral point is not a point of bifurcation.

It is of interest to recall that in the case of the Maclaurin spheroids, the corresponding neutral point is a point of bifurcation.[28] At this point a sequence of pear-shaped configurations branches off from the sequence of spheroids. The absence of this sequence of pear shapes along the axisymmetric sequence for the rotating charged liquid drop clearly depends upon the presence of the surface tension. Whether this conclusion also depends critically upon the assumed spheroidal shapes cannot be decided within the present considerations.

B. Equations of Odd Parity

The eight equations of odd parity correspond to Eqs. (36)–(43) of Ref. 22. These equations can be arranged into a form corresponding to Eqs. (87)–(94) of Ref. 22. In this latter form, the quantity $\delta\Pi_3$ can be eliminated. In the present case of axisymmetry, the resulting equations separate into two noncombining groups.

The first group (hereafter called Group F) contains the four equations

$$\lambda^2 V_{3;12} + Q_1 V_{123} = 0, \tag{132}$$

$$\lambda^2(V_{3;11} - V_{3;22}) + Q_1(V_{311} - V_{322}) = 0, \tag{133}$$

$$\lambda^2(V_{1;23} + V_{2;31}) + 2\lambda\Omega(V_{1;31} - V_{2;32}) + (Q_1 + Q_2 - 2\Omega^2)V_{123} = 0, \tag{134}$$

$$2\lambda^2(V_{1;31} - V_{2;32}) - 4\lambda\Omega(V_{1;23} + V_{2;31}) + (Q_1 + Q_2 - 2\Omega^2)(V_{311} - V_{322}) = 0, \tag{135}$$

where

$$Q_1 = (T/\rho)[7(\mathfrak{A}_{13} - 2\mathfrak{B}_{113}) - (2\sigma^2/T)(B_{13} + a_1^2 B_{113})], \quad (136)$$

$$Q_2 = (T/\rho)[7(\mathfrak{A}_{11} - 2\mathfrak{B}_{113}) - (2\sigma^2/T)(B_{11} + a_3^2 B_{113})]. \quad (137)$$

The remaining three equations depend upon the divergence condition

$$a_1^{-2}(V_{311} + V_{322}) + a_3^{-2} V_{333} = 0, \quad (138)$$

which can be used to eliminate V_{333}. Then the second group (hereafter called Group G) can be written in the form

$$\lambda^2(V_{1;23} - V_{2;31}) - 2\lambda\Omega(V_{1;31} + V_{2;32}) = 0, \quad (139)$$

$$\lambda^2(V_{3;11} + V_{3;22}) + Q_3(V_{311} + V_{322}) = 0, \quad (140)$$

$$2\lambda^2(V_{1;31} + V_{2;32}) + 4\lambda\Omega(V_{1;23} - V_{2;31}) + [(a_3^2/a_1^2)(\tfrac{2}{3}\lambda^2 + Q_4) + Q_3 - Q_5 - 2\Omega^2] \times (V_{311} + V_{322}) = 0, \quad (141)$$

where

$$Q_3 = (5T/\rho)[7\mathfrak{B}_{133} - (\sigma^2/T)(B_{13} - a_3^2 B_{133})], \quad (142)$$

$$Q_4 = \tfrac{1}{2}(T/\rho)[7(\mathfrak{A}_{13} + 25\mathfrak{B}_{133}) - (8\sigma^2/T)(4B_{13} - 5a_3^2 B_{133})], \quad (143)$$

and

$$Q_5 = \tfrac{1}{2}(T/\rho)[7(\mathfrak{A}_{13} - 5\mathfrak{B}_{133}) - (2\sigma^2/T)(B_{13} - 5a_3^2 B_{133})]. \quad (144)$$

1. Group F

The equations in Group F depend upon the quantities $V_{3;11} - V_{3;22}$, $V_{1;31} - V_{2;32}$, $V_{1;21} + V_{2;31}$, and $V_{3;12}$. The characteristic equation for these modes is

$$\lambda^2[\lambda^2(\lambda^2 + 2Q_1 + Q_2 - 2\Omega^2)^2 + 4\Omega^2(\lambda^2 + Q_1)^2] = 0. \quad (145)$$

In addition to the factor λ^2, Eq. (145) contains a polynomial of degree three in λ^2. If we replace λ^2 by $-\omega^2$, then this polynomial can be written as the product of two cubic factors. We have

$$\omega^3 \pm 2\Omega\omega^2 - (2Q_1 + Q_2 - 2\Omega^2)\omega \mp 2\Omega Q_1 = 0. \quad (146)$$

It follows from Eq. (146) that a neutral mode ($\omega = 0$) obtains when

$$Q_1 = 0. \quad (147)$$

However, this neutral mode does not indicate the occurrence of a point of bifurcation. It is impossible to simultaneously satisfy Eq. (147), the relation

$$2\Omega^2 = Q_2, \quad (148)$$

and Eq. (38) (the equilibrium relation), and all three of these relations are necessary conditions for the occurrence of a point of bifurcation.

2. Group G

The equations in Group G depend upon the quantities $V_{3;11} + V_{3;22}$, $V_{1;31} + V_{2;32}$, and $V_{1;23} - V_{2;31}$. If we replace λ^2 by $-\omega^2$, then the characteristic equation assumes the form

$$\omega^2\{(\tfrac{2}{3} + \alpha)\omega^4 - [\alpha(2\Omega^2 + 2Q_3 - Q_5) + Q_4]\omega^2 + 4\alpha\Omega^2 Q_3\} = 0. \quad (149)$$

Although a neutral mode obtains when

$$Q_3 = 0, \quad (150)$$

it does not indicate the occurrence of a point of bifurcation.

The characteristic equations (146) and (149) are of the same form as Eqs. (25) and (27) of Ref. 27, so that the odd modes in this case and in the case of the Maclaurin spheroids behave in a similar fashion.

There are a total of 11 nonvanishing values of ω^2 in the third order, in agreement with a lemma of Cartan.[26]

VII. NUMERICAL RESULTS, DISCUSSION, AND SUMMARY

The foregoing investigation of the stability of a rotating charged liquid drop has been restricted to those equilibrium configurations which initially have triplanar symmetry, and in particular to those which are axisymmetric. Under these restrictions, all of the equilibrium relations, provided by the virial equations through the third order (a total of 30), are satisfied when Eqs. (30) and (31) are satisfied. We have evaluated these relations by assuming that the equilibrium configurations are spheroids. These spheroids must rotate about the axis of symmetry. The appropriate values of charge and angular momentum that should be associated with a spheroid having a given eccentricity are defined by Eqs. (38) and (40). Additional formulas were derived which indicated the occurrence of points of bifurcation where new sequences of equilibrium configurations branch off from the sequences of spheroids.

The numerical evaluation of all the formulas is greatly facilitated by the use of the algebraic recursion relations among the multi-index symbols. Once the numerical values of the one-index symbols $\mathfrak{A}_1$, $\mathfrak{A}_3$, A_1, and A_3 are known, all of the index symbols with more than one index can be evaluated by using the relations derived in Refs. 18 and 19. The one-index symbols are evaluated (in these references) in terms of elementary functions. The resulting expressions depend only upon the eccentricity of the spheroid.

The formulas to be evaluated also involve the important parameters σ^2/T and $\rho\Omega^2/2T$ (in our units). When the supressed constants are restored (Appendix B), we find that σ^2/T represents the fissionability parameter x, and $\rho\Omega^2/2T$ represents the rotational parameter y, of nuclear fission theory. These parameters are dimensionless ratios of energies. The parameter x measures the relative importance of the electrostatic energy to the surface energy, and the parameter y measures the relative importance of the rotational energy to the surface energy. It is convenient to express the results of the following discussion in terms of these parameters.

Sequences of both oblate and prolate spheroids satisfy the equilibrium equations. For each of these classes of figures, we shall delineate the extent of the equilibrium sequences and locate the points of bifurcation. The appropriate physical interpretation of each class of figures then follows from a closer examination of the stability. We shall also indicate the limits within which the spheroids approximate the exact figures of equilibrium. Some additional qualitative conclusions concerning the exact figures will be inferred.

A. Oblate Spheroids ($a_3 < a_1$)

The eccentricity of an oblate spheroid is

$$e = (1 - a_3^2/a_1^2)^{\frac{1}{2}}. \tag{151}$$

For a given value of e, Eq. (38) defines a linear relationship between x and y. Some representative lines of constant e are shown in Fig. 1. As the rotational energy is increased for a given charge, an increased mean surface curvature is required at the equator to provide the added pressure needed to balance the additional centrifugal force. Therefore, a sequence of spheroids with increasing e is generated by increasing y for a given value of x. The centrifugal force is relatively more effective in deforming the drop for large values of x, where the surface tension and the electrostatic forces nearly balance already. Hence all the lines of constant e have negative slopes. The lines all have x intercepts greater than $x = 1$. Since the lines never cross, each point (x, y) in Fig. 1 is associated with a single oblate spheroid. However, the same oblate spheroid may be associated with any value of (x, y) along a given line of constant e. In the limit that y approaches zero, these families of oblate spheroids merge with the family of nonrotating, spherical equilibrium configurations defined for $0 \leq x < 1$. (Further discussion of the nonrotating configurations is given in Appendix E.)

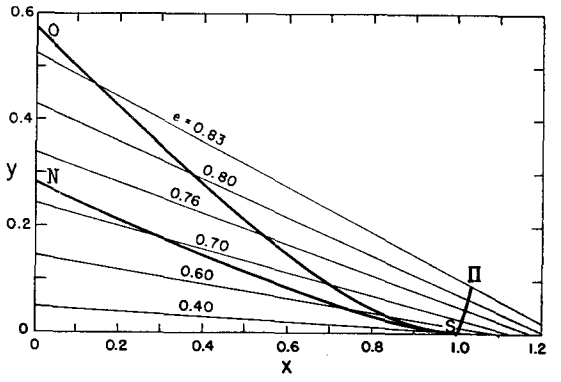

FIG. 1. The variation of x and y with the eccentricity e of rotating oblate spheroids (ground states). Allowed equilibrium configurations lie between the curves $x = 0$ and ΠS. Configurations which are stable with respect to second harmonics lie below the curve of overstability OS. Along the curve of neutral stability NS, tri-axial ellipsoids first become possible equilibrium configurations.

It is well known that when x exceeds 1, the attractive surface tension is no longer sufficient to hold a spherical drop together against the repulsive electrostatic forces. For these values of x, the volume integral of the internal pressure, which we have denoted by Π, is no longer positive. So in general, the extent of the allowed rotating oblate equilibrium configurations beyond $x = 1$ is limited by the curve ΠS in Fig. 1 along which Π vanishes. This curve follows from Eq. (40). Only those configurations whose x and y are to the left of this curve are admissible equilibrium configurations.

Some additional lines of constant e are defined by the parameters in Table I. Other parameters have been given by Beringer and Knox.[8]

When the equilibrium relations are satisfied, we may proceed with the investigation of the stability of the equilibrium configurations. The analysis of the characteristic frequencies belonging to the second harmonics has revealed the presence of a neutral point along a sequence of axisymmetric equilibrium configurations. In the case of spheroids, the parametric equations (75) and (76) determine the values of x and y at which a given spheroid

TABLE I. The x and y intercepts of the lines of constant eccentricity e in the case of oblate spheroids in equilibrium. The values of x and y along the limiting curve ΠS are included.

e	Intercepts		ΠS	
	y	x	x	y
0.40	0.05031	1.02648	1.00086	0.00126
0.50	0.08738	1.04545	1.00232	0.00360
0.55	0.11308	1.05834	1.00362	0.00585
0.60	0.14565	1.07441	1.00553	0.00934
0.64	0.17837	1.09026	1.00767	0.01351
0.67	0.20808	1.10443	1.00976	0.01784
0.70	0.24354	1.12108	1.01240	0.02361
0.72	0.27121	1.13388	1.01455	0.02854
0.74	0.30288	1.14834	1.01708	0.03462
0.76	0.33946	1.16481	1.02008	0.04218
0.78	0.38216	1.18374	1.02365	0.05168
0.80	0.43263	1.20572	1.02795	0.06379
0.81	0.46146	1.21812	1.03042	0.07110
0.82	0.49317	1.23161	1.03315	0.07947
0.83	0.52823	1.24636	1.03618	0.08908
0.84	0.56718	1.26257	1.03955	0.10019
0.85	0.61073	1.28048	1.04331	0.11312
0.86	0.65996	1.30039	1.04753	0.12829
0.87	0.71540	1.32267	1.05230	0.14623
0.88	0.77912	1.34781	1.05772	0.16769

admits a neutral mode of this type. Each allowed sequence of oblate spheroids admits this neutral mode at a different point; the resulting curve of neutral stability NS is shown in Fig. 1.

This neutral point is also a point of bifurcation where genuine tri-axial figures are expected to become possible figures of equilibrium. Each point along the curve NS indicates the values of x and y belonging to the first member of a sequence of ellipsoidal figures of equilibrium (see Appendix C). When taken together for all values of x, these sequences form a "second sheet" of equilibrium figures in the region of the plane above the curve NS.

In the absence of any dissipative mechanism, the spheroidal figures continue to be stable beyond this neutral point. When Eqs. (79) and (80) are satisfied, the oscillation frequencies for the γ vibration finally become complex. The resulting curve of overstability OS is shown in Fig. 1. For values of y above this curve, oblate spheroids are unstable with respect to the γ vibration.

TABLE II. The variation of the rotational parameter y, the deformation energy ξ, and the eccentricity e with the fissionability parameter x along the curves of neutral stability and overstability resulting from the γ vibration of oblate spheroids.

x	Neutral Stability			Overstability		
	y	$\xi \times 10$	e	y	$\xi \times 10$	e
0.0000	0.2830	−0.3605	0.72775	0.5795	−1.2073	0.84295
0.1000	0.2481	−0.3080	0.72058	0.4990	−1.0008	0.83374
0.2000	0.2137	−0.2571	0.71202	0.4209	−0.8087	0.82269
0.3000	0.1799	−0.2084	0.70158	0.3458	−0.6300	0.80917
0.4000	0.1469	−0.1622	0.68854	0.2742	−0.4675	0.79219
0.5000	0.1150	−0.1193	0.67173	0.2069	−0.3239	0.77016
0.6000	0.0844	−0.0804	0.64909	0.1450	−0.2025	0.74035
0.7000	0.0558	−0.0469	0.61664	0.0900	−0.1067	0.69746
0.8000	0.0302	−0.0207	0.56520	0.0446	−0.0406	0.62986
0.9000	0.0097	−0.0043	0.46660	0.0125	−0.0067	0.50446
1.0000	0.0000	0.0000	0.00000	0.0000	0.0000	0.00000

Table II contains values of y and e along the curves NS and OS as functions of x. The values for the curve NS agree with those obtained by Carlson and Pao Lu,[9] by Pik-Pichak,[29] and by Cohen, Plasil, and Swiatecki.[10] We have also tabulated the deformation energy, which is defined in Appendix C.

An examination of Eqs. (83) and (91) reveals that the oblate spheroids do not become unstable with respect to either of the other two modes belonging to the second harmonics. Therefore, we conclude that the oblate spheroids are completely *stable* with respect to second-harmonic deformations throughout the entire triangular region bounded by the x and y axes and by the curve OS. This means that we may tentatively identify the oblate axisymmetric figures of equilibrium as a class of rotating ground-state configurations. This would certainly be the case if these configurations are also stable with respect to all the deformations belonging to higher harmonics.

It is of interest to justify the use of oblate spheroids in our investigation of the stability of the exact axisymmetric configurations and to establish the range over which this approximation is valid. Unfortunately, closed expressions for the exact figures of equilibrium of a rotating charged liquid drop are unknown. However, in the limit of zero charge ($x = 0$), the exact axisymmetric figures of equilibrium are known. The neutral and overstable points belonging to the second harmonics were obtained for these exact configurations by Chandrasekhar[23] using the virial method. An indication of the error committed in using oblate spheroids instead of the exact figures can be obtained by comparing the values of y corresponding to the neutral and overstable points in the two cases.

When $x = 0$, it follows from Eq. (75) that

$$\mathcal{A}_{11} = e^2 \mathcal{A}_{13}. \tag{152}$$

By using the expressions for the multi-index symbols derived in Ref. 18, Eq. (152) reduces to

$$\frac{\tanh^{-1} e}{e} = \frac{3 + 12e^2 - 7e^4}{(1 - e^2)(3 + 4e^2 + 7e^4)}. \tag{153}$$

The solution of Eq. (153) is $e = 0.727754$. Thus,

[29] G. A. Pik-Pichak, Zh. Eksperim. i Teor. Fiz. 43, 1701 (1962) [English transl.: Soviet Phys.—JETP 16, 1201 (1963)].

our neutral point occurs when $y = 0.28297$. This is to be compared with Chandrasekhar's more exact value: $y = 0.28338$ (his $\Sigma = 0.45871$).[30]

It follows from Eq. (79) that the point of overstability in the limit of zero charge obtains when

$$2\mathcal{A}_{11} = e^2\mathcal{A}_{13}. \tag{154}$$

This equation reduces to

$$\frac{\tanh^{-1} e}{e} = \frac{3 + 6e^2 - 5e^4}{(1 - e^2)(3 + 8e^2 + 5e^4)}. \tag{155}$$

The solution of Eq. (155) is $e = 0.842948$. Therefore, our overstable oscillations begin when $y = 0.57951$. This is to be compared with Chandrasekhar's more exact value of $y = 0.5930$ (his $\Sigma = 0.84404$).

Thus, up to the overstable point in the limit of zero charge, this comparison shows that the error in using spheroids to estimate the exact critical values of y is less than 3%. In this limit, the value obtained for y is consistently *less* than the more exact value, with the error increasing as y increases.

On the other hand, in the neighborhood of $x = 1$, the critical values of y, obtained by using spheroids, are consistently *greater* than the more exact values. This follows from a comparison of the leading correction terms in series expansions for the critical curves in this limit. For the curve NS, we obtain

$$y = \tfrac{7}{5}(1 - x)^2[1 - \tfrac{9}{2}(1 - x) + \cdots], \qquad 0 < 1 - x \ll 1 \tag{156}$$

for spheroids. This agrees with the expansion obtained by Pik-Pichak,[29] who also obtained[31] a more exact expansion

$$y = \tfrac{7}{5}(1 - x)^2[1 - \tfrac{504}{85}(1 - x) + \cdots]. \tag{157}$$

For the curve of overstability OS, we obtain

$$y = \tfrac{7}{5}(1 - x)^2[1 - (1 - x) + \cdots], \qquad 0 < 1 - x \ll 1 \tag{158}$$

for spheroids. A more exact expansion has not yet been obtained for this curve.

Beyond the curve of overstability, the error in using spheroids rapidly increases. In the limit of zero charge, the exact figures of equilibrium begin to develop a dimple in the polar regions when y exceeds 0.74305 ($\Sigma = 1$). This corresponds to an eccentricity $e = 0.87451$. Beyond this eccentricity, the spheroids are not expected to be adequate approximations to the exact figures of equilibrium.

Among the oscillations belonging to the third harmonics, only those belonging to Group D indicated the occurrence of a point of bifurcation along a sequence of spheroidal configurations. When Eqs. (114) and (115) are satisfied, we may expect asymmetric configurations to become possible figures of equilibrium. The spheroids cease to be stable with respect to the asymmetric deformation (121) when Eqs. (38) and (117) are simultaneously satisfied. Unfortunately, the values of eccentricity which satisfy these equations are beyond the expected limit of validity of $e = 0.87451$. When the numerator of Eq. (114) vanishes in the limit of zero charge, we obtain the relation

$$\frac{\tanh^{-1} e}{e} = \frac{105 - 70e^2 + 79e^4 - 66e^6}{(1 - e^2)(105 + 93e^4 + 66e^6)}. \tag{159}$$

The solution of this equation is $e = 0.87997$, which corresponds to a value of $y = 0.77892$. A similar calculation indicates that when $x = 0$, the spheroids become overstable with respect to this mode when $e = 0.92211$. The corresponding value of y is 1.1968. The third neutral point along a sequence of spheroids (the one which does not appear to be a point of bifurcation) obtains when Eqs. (38) and (128) are simultaneously satisfied. This occurs in the limit of zero charge when $e = 0.95594$ and $y = 1.9869$.

Since these critical values are all beyond the limit of validity, further quantitative estimates of the stability with respect to the third-harmonic oscillations, which are based on the spheroidal approximation, are expected to be greatly in error. However, several qualitative conclusions concerning the exact axisymmetric configurations can still be inferred. The virial equations for the exact configurations are expected to separate formally into the four symmetry Groups D, E, F, and G. As in the case of Group A (in the second order), Group D, which exhibits a point of bifurcation here, is independent of the divergence condition, and therefore is relatively insensitive to the particular properties of a shape which already possesses the proper symmetry. This implies that the exact axisymmetric configurations will also exhibit these points of bifurcation and overstability. Moreover, for a given value of x, the point of bifurcation resulting from the third-harmonic deformation may be expected to occur for a greater value of y than the point of bifurcation resulting from the second-harmonic deformation. (It may, however, occur before the configurations become overstable with respect to second harmonics, as is the case for the Maclaurin

[30] His $\Sigma = \rho\Omega^2a^3/8T$, where a is the equatorial radius of the drop, is closely related to our y; see Appendix B.

[31] G. A. Pik-Pichak, Zh. Eksperim. i Teor. Fiz. **42**, 1294 (1962) [English transl.: Soviet Phys.—JETP **15**, 897 (1962)].

spheroids.) This supports the view that the lower harmonics may be considered first in an investigation of stability.

B. Prolate Spheroids ($a_3 > a_1$)

The eccentricity of a prolate spheroid is

$$k = (1 - a_1^2/a_3^2)^{\frac{1}{2}}. \tag{160}$$

For a given value of k, Eq. (38) defines a linear relation between x and y. Some representative lines of constant k are shown in Fig. 2. All of the lines have a positive slope. (The existence of the rotating prolate spheroids was first pointed out by Hiskes.[7])

The extent of the allowed configurations beyond $x = 1$ is limited by the restriction of Π to positive values. Only those configurations with x and y values to the left of the curve $\Pi'S$, along which Π vanishes, are admissible equilibrium configurations.

The rotating prolate spheroids do not fill the entire allowed region of the x, y plane, but exist only in a small neighborhood around $x = 1$. Initially, as k increases from zero, the families of spheroids form a sheet of allowed configurations. When k reaches the value 0.901 which corresponds to $x = 0.886$, this sheet "turns back" or folds back on itself forming a second sheet which overlaps the first. The behavior of turning back was also exhibited by the original nonrotating Bohr–Wheeler saddle shapes.[2] (Indeed, by using the x intercepts of these lines of constant k, the known equilibrium curve associated with nonrotating spheroids can be obtained. See Appendix E.)

Positive identification of these figures as saddle shapes follows from an examination of their stability. All of the rotating prolate spheroids are unstable ($\omega^2 < 0$) with respect to the β vibration described by the equations in Group B. This represents the fission mode along the axis of symmetry (which in this case also coincides with the axis of rotation). In addition, the rotating prolate spheroids are overstable (ω complex) with respect to the transverse-shear mode (Group C) for $k < 2(\frac{2}{3})^{\frac{1}{2}}$. For greater values of k the spheroids are stable with respect to this mode.

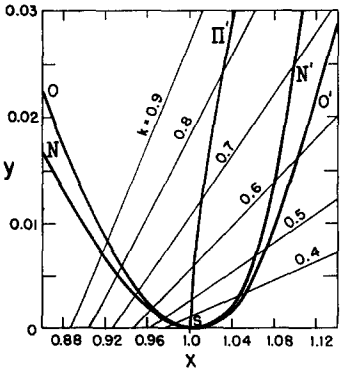

FIG. 2. The variation of x and y with the eccentricity k of prolate spheroids (saddle shapes) which rotate about the symmetry axis. Allowed equilibrum configurations lie to the left of the curve $\Pi'S$. The curves of neutral stability and overstability for both prolate ($N'S$, $O'S$) and oblate (NS, OS) spheroids are shown.

The curves of neutral stability $N'S$ and overstability $O'S$, which obtained from Eqs. (75), (76), (79) and (80) in the case of prolate spheroids, lie in the unphysical region containing the equilibrium configurations with negative Π. The unphysical sequences (x = const) in this region are initially overstable with respect to the γ vibration. When y has been increased to $O'S$, the oscillation frequencies for this mode become real. Later, along $N'S$, a neutral mode occurs which indicates a point of bifurcation. The sequences of ellipsoidal figures, which coincide with the sequences of spheroidal figures along $N'S$, must have, initially, negative values of Π. For comparison with Fig. 1, the curves NS and OS for oblate spheroids are also shown in Fig. 1.

The prolate spheroids are not a good approximation for this particular class of rotating saddle shapes. This conclusion follows from a comparison of these figures with the more exact figures obtained by Cohen and Swiatecki[3] in the limit of zero charge. Their studies have shown that the behavior of turning back, exhibited here by the nonrotating prolate spheroids, was not exhibited by their more exact figures of equilibrium (see Appendix E). Moreover, it is clear from their calculations and earlier series expansions that the nonrotating prolate spheroids with $k > 0.5$ no longer closely approximate the more exact configurations. Qualitatively, this simply means that higher moments of the surface (and in particular the fourth moments) are not unimportant. Therefore, further quantitative analysis using prolate spheroids is expected to be greatly in error.

We have employed approximate figures of equilibrium and approximate proper solutions in these investigations of stability. In those regions where the exact figures of equilibrium are adequately approximated by spheroids, the oscillation frequencies obtained by using the trial displacement (52) are moderately accurate. This aspect of the virial method resembles the solution of a characteristic value problem by a variational method. In addition, the virial method shows that the qualitative aspects of bifurcation and overstability, exhibited here in the case of spheroids, can be expected to occur in a similar manner in the case of more exact axisymmetric figures of equilibrium.

ACKNOWLEDGMENT

The author wishes to thank Professor S. Chandrasekhar for his advice during the progress of this work.

APPENDIX A. POTENTIAL-ENERGY TENSORS OF HOMOGENEOUS ELLIPSOIDS

In view of the formal similarity between gravitation and electrostatics, all of the formalism, previously developed by Chandrasekhar and Lebovitz in the content of gravitation, can be used here to evaluate the electrostatic potential-energy tensors of homogeneously charged ellipsoids. After comparing the formulas in Appendix A of Ref. 14 with those in Ref. 19, the correct expressions for charged ellipsoids can be obtained. (Note that the signs of the potential-energy tensors change, while those of the potentials remain unchanged.) We have (no summation over repeated indices)

$$(\pi\sigma a_1a_2a_3)^{-1}\mathfrak{W}_{ij} = 2B_{ij}x_ix_j + a_i^2\,\delta_{ij}\,[A_i - (A_{i1}x_1^2 + A_{i2}x_2^2 + A_{i3}x_3^2)], \tag{A1}$$

$$\mathfrak{W}_{ii} = (8\pi^2\sigma^2/15)(a_1a_2a_3)^2a_i^2A_i \tag{A2}$$

$$= 2\sigma^2a_i^2A_i \qquad \text{(our units)}, \tag{A3}$$

$$\delta\mathfrak{W}_{ij} = (2\sigma^2/\rho)B_{ij}V_{ij} \qquad (i \neq j), \tag{A4}$$

and

$$\delta\mathfrak{W}_{ii} = (\sigma^2/\rho)[(3B_{ii} - A_i)V_{ii} + (B_{ij} - A_i)V_{ij} + (B_{ik} - A_k)V_{kk}] \qquad (i \neq j \neq k), \tag{A5}$$

where A_i, B_{ij}, and B_{ii} are the multi-index symbols defined in Ref. 13.

The correct expressions for $\delta\mathfrak{W}_{ij;k}$ can be obtained directly from Eqs. (119)–(122) of Ref. 22 or from Table 1 of Ref. 22, by replacing the suppressed factor $\pi G\rho a_1a_2a_3$ with the factor $-\pi\sigma^2a_1a_2a_3/\rho$ which becomes just $-\sigma^2/\rho$ in our units. The appropriate formulas for spheroids ($a_1 = a_2$) are given in Tables 1-3 of Ref. 27, with the same convention as above regarding the suppressed factor.

APPENDIX B. PARAMETERS x AND y

In nuclear physics the equilibrium configurations of a rotating charged liquid drop are usually classified in terms of the fissionability parameter x and the rotational parameter y. These parameters are, respectively, the dimensionless ratios of one-half the Coulomb energy E_c^0 and of the rotational energy E_r^0 to the surface energy E_s^0. The superscript zero implies that all these quantities refer to a reference *sphere* of radius R. This reference sphere has the same surface tension T, the same uniformly distributed total charge Q, the same uniformly distributed total mass, and the same total volume as the actual equilibrium configuration. In addition, this sphere is rigidly rotating with the same angular momentum $\mathfrak{M}$ as the actual equilibrium configuration.

The fissionability parameter can be written in several forms. We have

$$x = \frac{E_c^0}{2E_s^0} = \frac{(3Q^2)/(5R)}{2T(4\pi R^2)} = \frac{Q^2}{10T(4\pi R^3/3)} = \frac{2\pi\sigma^2R^3}{15T}, \tag{B1}$$

and in terms of the atomic number Z and the mass number A,

$$x = (Z^2/A)(Z^2/A)_{\text{crit}}^{-1}, \tag{B2}$$

where $(Z^2/A)_{\text{crit}}$ is an empirical constant. Throughout this paper, the quantity σ^2/T in our units represents x. By restoring the suppressed constants, we have

$$\left(\frac{\sigma^2}{T}\right)_{\text{our units}} = \frac{\sigma^2[4\pi^2(a_1a_2a_3)^2/15]}{T[\pi(a_1a_2a_3)^2]} = \frac{4\pi\sigma^2}{15T} = \frac{2x}{R^3}. \tag{B3}$$

Since the reference sphere and the actual equilibrium configuration have the same angular momentum, it follows that

$$|\mathfrak{M}|^2 = (\Omega^0I^0)^2 = (\Omega I)^2, \tag{B4}$$

where Ω and

$$I = I_{11} + I_{22} \tag{B5}$$

are, respectively, the angular velocity and the moment of inertia of the actual equilibrium configuration about its axis of rotation. By using Eq. (B4), we can express the rotational parameter in the form

$$y = \frac{E_r^0}{E_s^0} = \frac{|\mathfrak{M}|^2}{2I^0E_s^0} = \tfrac{1}{2}\Omega^2\left(\frac{I}{I^0}\right)^2\left(\frac{I^0}{E_s^0}\right) = \frac{\rho\Omega^2}{15T}\left(\frac{I}{I^0}\right)^2R^3. \tag{B6}$$

Throughout this paper, the quantity $\rho\Omega^2/2T$ in our units represents y. By restoring the suppressed constants, we have

$$\left(\frac{\rho\Omega^2}{2T}\right)_{\text{our units}} = \frac{\rho\Omega^2[4\pi(a_1a_2a_3)/15]}{2T[\pi(a_1a_2a_3)^2]} = \frac{2\rho\Omega^2}{15T(a_1a_2a_3)} = \frac{2y}{R^6}\left(\frac{I^0}{I}\right)^2. \tag{B7}$$

In writing these formulas, we have made use of the relation (valid for ellipsoids)

$$R^3 = a_1 a_2 a_3. \tag{B8}$$

For the cases considered in this paper

$$I/I^0 = (a_1^2 + a_2^2)/2R^2. \tag{B9}$$

One further dimensionless parameter is useful in connection with studies of the liquid drop. This parameter is the deformation energy and is given the symbol ξ. (This symbol should not be confused with our Lagrangian displacements.) It is a measure of the energy difference between the actual figure of equilibrium and the associated reference sphere defined above. In our notation

$$\xi = (E_s^0)^{-1}(\mathfrak{W} + \mathfrak{S} + |\mathfrak{M}|^2/2I) - (2x + y + 1). \tag{B10}$$

For ellipsoids, we have

$$\begin{aligned}\xi = {} & x[(a_1a_2a_3)^{\frac{1}{3}}(a_1^2A_1 + a_2^2A_2 + a_3^2A_3) - 2] \\ & + y[2(a_1a_2a_3)^{\frac{1}{3}}(a_1^2 + a_2^2)^{-1} - 1] \\ & + [\tfrac{1}{2}(a_1a_2a_3)^{4/3}(\mathfrak{A}_1 + \mathfrak{A}_2 + \mathfrak{A}_3) - 1].\end{aligned} \tag{B11}$$

A more complete discussion of the relationship between the fission barriers and other energies associated with rotating and nonrotating liquid drops has been given by Plasil.[11]

APPENDIX C. ROTATING ELLIPSOIDS

In order to demonstrate that sequences of triaxial ellipsoids do bifurcate from sequences of spheroids at the values of σ^2/T and $\rho\Omega^2/2T$ indicated by Eqs. (75) and (76), we first obtain the values of σ^2/T and $\rho\Omega^2/2T$ which define the sequences of ellipsoids ($a_1 \neq a_2$) and then pass to the limit $a_1 = a_2$ in order to recover Eqs. (75) and (76).

For this purpose, it is convenient to form the sum and difference of Eqs. (36) and (37), which hold generally for ellipsoids. We have

$$\begin{aligned}&(\rho\Omega^2/2T)(a_1^2 + a_2^2) + (\sigma^2/T) \\ &\quad \times [(a_1^2A_1 - a_3^2A_3) + (a_2^2A_2 - a_3^2A_3)] \\ &\quad = (\mathfrak{A}_3 - \mathfrak{A}_1) + (\mathfrak{A}_3 - \mathfrak{A}_2)\end{aligned} \tag{C1}$$

and

$$\begin{aligned}&(\rho\Omega^2/2T)(a_1^2 - a_2^2) \\ &\quad + (\sigma^2/T)(a_1^2A_1 - a_2^2A_2) = \mathfrak{A}_2 - \mathfrak{A}_1.\end{aligned} \tag{C2}$$

These equations may be rearranged by using the definitions of the two-index symbols to obtain

$$\begin{aligned}&(\rho\Omega^2/2T)(a_1^2 + a_2^2) \\ &\quad + (\sigma^2/T)[(a_1^2 - a_3^2)B_{13} + (a_2^2 - a_3^2)B_{23}] \\ &\quad = (a_1^2 - a_3^2)\mathfrak{A}_{13} + (a_2^2 - a_3^2)\mathfrak{A}_{23}\end{aligned} \tag{C3}$$

and

$$(\rho\Omega^2/2T) + (\sigma^2/T)B_{12} = \mathfrak{A}_{12}. \tag{C4}$$

We can solve Eqs. (C3) and (C4) for

$$\frac{\sigma^2}{T} = \frac{(a_1^2 + a_2^2)\mathfrak{A}_{12} - (a_1^2 - a_3^2)\mathfrak{A}_{13} - (a_2^2 - a_3^2)\mathfrak{A}_{23}}{(a_1^2 + a_2^2)B_{12} - (a_2^2 - a_3^2)B_{13} - (a_2^2 - a_3^2)B_{23}} \tag{C5}$$

and

$$\frac{\rho\Omega^2}{2T} = \frac{(a_1^2 - a_3^2)(\mathfrak{A}_{13}B_{12} - \mathfrak{A}_{12}B_{13}) + (a_2^2 - a_3^2)(\mathfrak{A}_{23}B_{12} - \mathfrak{A}_{12}B_{23})}{(a_1^2 + a_2^2)B_{12} - (a_1^2 - a_3^2)B_{13} - (a_2^2 - a_3^2)B_{23}}. \tag{C6}$$

Equations (C5) and (C6) determine the equilibrium values of σ^2/T and $\rho\Omega^2/2T$ for ellipsoids when the ratios a_2/a_1 and a_3/a_1 are given.

The limiting forms of Eqs. (C5) and (C6), which are appropriate for a spheroid at the beginning of the sequence, can be obtained by replacing the index 2 by the index 1 wherever it appears in these equations. The resulting expressions are exactly Eqs. (75) and (76).

Here, we have obtained the first point of bifurcation along the sequence of spheroids by using only *equilibrium* relations. This was possible because the exact form of the new figure was already known. It is important to realize that Eqs. (75) and (76), which give the locus of instability, cannot be determined by a similar argument. The full normal mode analysis was necessary for their determination and interpretation.

APPENDIX D. REARRANGEMENT OF GROUP E

The equation

$$\begin{aligned}&(\lambda^2 - \Omega^2)V_{133} - (\tfrac{1}{3}\lambda^2 - \Omega^2)V_{111} \\ &\quad - 2\lambda\Omega(V_{2;33} - V_{2;11}) + \delta\mathfrak{U}_{133} = 0\end{aligned} \tag{D1}$$

corresponds to Eq. (60) of Ref. 22. The quantity $\delta\mathfrak{U}_{133}$ can be expanded in the form

$$\delta\mathfrak{U}_{133} = aV_{111} + bV_{122} + cV_{133}, \tag{D2}$$

where the coefficients a, b, c are computed from

the tables according to Eq. (93). Equation (D1) can be rearranged in the form

$$\tfrac{1}{4}[3(b-a) - 3\Omega^2 + \lambda^2](V_{122} - \tfrac{1}{3}V_{111}) - \tfrac{1}{4}[4c\alpha^{-1} - 3a - b - \Omega^2(3 + 4\alpha^{-1}) + \lambda^2(1 + 4\alpha^{-1})](V_{111} + V_{122}) + (c - \Omega^2 + \lambda^2)[V_{133} + \alpha^{-1}(V_{111} + V_{122})] - 2\lambda\Omega(V_{2;33} - V_{2;11}) = 0. \quad \text{(D3)}$$

In view of Eq. (99), the third term of Eq. (D3) vanishes and the second term is proportional to αV_{133}. By judicious use of the recursion relations for the multi-index symbols, the relations

$$3(b-a) = P_1 \quad \text{(D4)}$$

and

$$4c\alpha^{-1} - 3a - b = N_1 + (11 + 4\alpha^{-1})M_1 - 8(1 - \alpha^{-1})Q \quad \text{(D5)}$$

can be obtained. Equation (101) follows from Eq. (D3) after Eq. (90) is used to eliminate Q from Eq. (D5). Equations (103) and (105) can be obtained in a similar manner without the use of Eq. (90).

APPENDIX E. NONROTATING SPHEROID

The nonrotating charged liquid drop has been extensively investigated by Cohen and Swiatecki.[2,3] Their calculations indicate that the equilibrium configurations for this case are not closely approximated by spheroids except in the neighborhood of $x = 1$. Nevertheless, for purposes of interpretation and clarification, it is instructive to recover the formulas appropriate for nonrotating spheroids from those appropriate for rotating spheroids by passing to the limit $\Omega = 0$.

If we associate the index 3 with the axis of symmetry, then it follows from Eq. (38) that the equilibrium configurations are defined by

$$\sigma^2/T = \mathcal{C}_{13}/B_{13}. \quad \text{(E1)}$$

The quantity σ^2/T is still restricted by Eq. (40), which follows from the requirement that Π be positive.

The virial equations separate into groups which have even and odd parity with respect to the index 3. Among the equations of the second order, Group A (the γ vibration) contributes two values of

$$\omega^2 = 2P, \quad \text{(E2)}$$

Group B (the β vibration) contributes one value of

$$\omega^2 = 2(1 + 2a_3^2/a_1^2)^{-1}[M + (a_3^2/a_1^2)N], \quad \text{(E3)}$$

and Group C contributes two values of

$$\omega^2 = 2Q. \quad \text{(E4)}$$

However, in view of Eq. (E1), the quantity Q must vanish for oscillations about these figures of equilibrium. Therefore, the equations of even parity contribute the only three nonvanishing values of ω^2 belonging to the second harmonics.

There are seven nonvanishing values of ω^2 belonging to the third harmonics. Group D contributes two values of

$$\omega^2 = P_1, \quad \text{(E5)}$$

Group E contributes two values of

$$\omega^2 = \left(4 + \frac{a_1^2}{a_3^2}\right)^{-1}\left[\left(4 + 11\,\frac{a_1^2}{a_3^2}\right)M_1 + \frac{a_1^2}{a_3^2}N_1\right], \quad \text{(E6)}$$

Group F contributes two values of

$$\omega^2 = 2Q_1 + Q_2, \quad \text{(E7)}$$

and Group G contributes one value of

$$\omega^2 = (\tfrac{2}{3} + a_1^2/a_3^2)^{-1}[(a_1^2/a_3^2)(2Q_3 - Q_5) + Q_4]. \quad \text{(E8)}$$

Finally, by making use of the expressions for the multi-index symbols and by restoring the suppressed constants, we can recover the formulas appropriate for a sphere of radius $a_1 = a_3 = R$. We have the condition

$$\Pi = (\tfrac{8}{3}\pi)TR^2(1 - x) \geq 0. \quad \text{(E9)}$$

Equations (E2)–(E4) reduce to the five values of

$$\omega^2 = (8T/\rho R^3)(1 - x) \quad \text{(E10)}$$

belonging to the second harmonics, and Eqs. (E5)–(E8) reduce to the seven values of

$$\omega^2 = (30T/\rho R^3)(1 - \tfrac{4}{7}x) \quad \text{(E11)}$$

belonging to the third harmonics.

Equation (E1) determines the equilibrium value of x associated with each eccentricity. In Fig. 3, the curve $E'S$ is the sequence of prolate figures ($a_3 > R$), and the curve ES is the sequence of

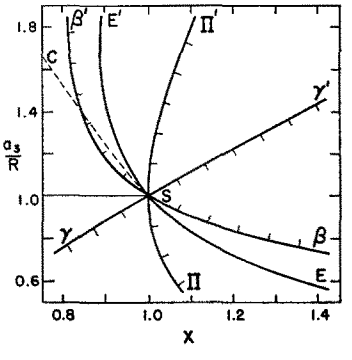

FIG. 3. Equilibrium curves E and limits of stability with respect to the γ and β vibrations of nonrotating prolate (symmetry axis $a_3 >$ radius of reference sphere R) and oblate spheroids. The shaded side of the curves is unstable or otherwise excluded. The dashed curve CS indicates the more exact saddle shapes of Cohen and Swiatecki.

oblate figures ($a_3 < R$). The allowed equilibrium configurations which have positive values of Π are restricted to the left side of the curve $\Pi' S \Pi$. This removes the oblate figures from further consideration. An examination of Eq. (E2), which determines the curve $\gamma S \gamma'$, reveals that the remaining prolate figures are stable ($\omega^2 > 0$) with respect to the γ vibration. However, Eq. (E3) and the curve $\beta' S$ reveal that the prolate figures are unstable ($\omega^2 < 0$) with respect to the β vibration, as is well known. The only stable region is the interior of the wedge $\beta' S \gamma$ which includes the line of stable spherical configurations. These spheres become unstable with respect to the second harmonics when x reaches the value 1. This same value of x represents the limit of possible spherical configurations in view of Eq. (E9).

The stable spherical figures correspond to ground-state configurations. The unstable prolate figures correspond to saddle shape configurations. They represent a first approximation (in the neighborhood of $x = 1$) to the original Bohr–Wheeler saddle shapes[1] and to the more exact saddle shapes [given by the dashed curve CS in Fig. 3] which were investigated by Cohen and Swiatecki.[2,3] The x intercepts of the equilibrium lines of constant k for the rotating prolate configurations in Fig. 2 reproduce the curve $E' S$ in Fig. 3. This illustrates how one may connect and identify the various classes of equilibrium configurations.

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Expanding Universe in Conformally Flat Coordinates*

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Einstein's field equations for a homogeneous isotropic universe are written in terms of a conformally flat coordinate system for both the closed and the open cases. It is shown that these can be readily integrated for equations of state of the form $p = a\rho$ in terms of algebraic functions. Explicit solutions and expressions for the radius and Hubble factor are given for $a = 1, \frac{1}{3}$, and for $p = 0$.

I. INTRODUCTION

In recent years there has been a renewed interest in the expanding universe, as originally formulated by Friedmann,[1] sparked to a large degree by the new observations in radio astronomy.[2] The characteristics of this universe are its isotropy and homogeneity expressed by the line element[3]

$$ds^2 = dT^2 - G^2\, d\sigma^2, \tag{1.1}$$

where $d\sigma^2 = g_{ij}\, dX^i\, dX^j$ ($i, j = 1, 2$, and 3) is the line element of a three-dimensional, homogeneous, and isotropic space with constant curvature, which can either be positive, zero, or negative, and is time independent. $G(T)$ is a function of the time T, measured by a clock comoving with the local nebula, and determined by the field equations and the equation of state.

The choice of the spatial coordinates is still arbitrary. A useful one for further work consists of introducing the dimensionless quantities

$$Y^i = X^i/R_0$$

and the radius

$$R = R_0 G,$$

which results in the isotropic form of the line element (1.1)

$$ds^2 = dT^2 - [G^2(T)/(1 + \tfrac{1}{4}kY^2)^2]\, d\mathbf{Y}\cdot d\mathbf{Y}, \tag{1.2}$$

where $k = 1, 0, -1$ depending on the sign of the curvature. Upon redefining the time T through

$$\tau = \int dT/R(T), \qquad R(T) = R(\tau),$$

we obtain the alternate form

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$$ds^2 = R^2\{d\tau^2 - [d\chi^2 + S^2(d\theta^2 + \sin^2\theta\, d\psi^2)]\}, \quad (1.3)$$

where

$$S(\chi) = \sin\chi(k = 1), \quad \sinh\chi(k = -1), \quad \chi(k = 0)$$

correspond to the transformation

$$Y = S(\chi).$$

Except in the simple cases corresponding to the dust-filled pressureless ($p = 0$) or constant density ($\rho = \text{const}$) universes, the solution of the field equations poses formidable mathematical difficulties.

In addition to being of interest in cosmological problems, (1.1) also has an important application to the implosion or explosion of spherically symmetric masses, where the interior solution is found to be identical to the elliptic cosmology corresponding to the line element (1.1).[4] Recently, equations of state of the form

$$p/c^2 = \alpha\rho \quad (1.4)$$

(α a constant) have been proposed to describe the elementary processes taking place in the interior of very condensed masses. Even in the simple case $\alpha = 1$, the solutions are given in terms of elliptic functions which have to be computed numerically for various values of the parameters.[5]

It would therefore be desirable to cast (1.1) into a form such that the field equations are readily integrable. Some time ago, Infeld and Schild[6] have shown that the postulates of constancy of the velocity of light, spatial isotropy, and homogeneity limit the possible types of universe to three, whose line element is conformal to the flat Minkowski space, and can be written as

$$ds^2 = F(s, t)\epsilon_{\mu\nu}\, dx^\mu\, dx^\nu, \quad (1.5)$$

where the function $F(s, t)$ must be one of the following forms, depending on the sign of the curvature:

$$k = 1, \quad F(s, t) = (1 - \tfrac{1}{4}s^2)^{-2} f[t/(1 - \tfrac{1}{4}s^2)], \quad (1.6a)$$

$$k = -1, \quad F(s, t) = (1 + \tfrac{1}{4}s^2)^{-2} f[t/(1 + \tfrac{1}{4}s^2)], \quad (1.6b)$$

$$k = 0, \quad F(s, t) = f(t), \quad (1.6c)$$

and $s^2 = t^2 - r^2$, $r^2 = x^2 + y^2 + z^2$, is the invariant distance.

Infeld and Schild have also shown that the conformal Minkowskian line element (1.5) is metrically, although not topologically, equivalent to the Robertson–Walker form (1.2). Introducing the variables[7]

$$2U = t + r, \quad 2V = t - r$$

and

$$2\xi = \tau + \chi, \quad 2\eta = \tau - \chi,$$

then, under the transformation

$$U = \tan\xi, \quad V = \tan\eta, \quad (1.7a)$$

(1.6a) transforms to the Robertson form corresponding to $k = 1$ with

$$R^2(\tau) = \sec^2\tau f(\tan\tau).$$

Similarily, for $k = -1$ the transformation

$$U = \tanh\xi, \quad V = \tanh\eta \quad (1.7b)$$

yields the corresponding form with

$$R^2(\tau) = \operatorname{sech}^2\tau f(\tanh\tau).$$

The third case, corresponding to $k = 0$, is not of interest for our work here, but it is listed for completeness. The required transformation is given by

$$U = 2\xi, \quad V = 2\eta, \quad (1.7c)$$

and results in

$$R^2(\tau) = f(\tau).$$

For the open universe ($k = -1$) the conformal factor $F(s, t)$ may be replaced by the simpler form

$$F(s, t) = e^{\Gamma(s)}, \quad (1.6d)$$

since under the transformation

$$U = e^{2\xi}, \quad V = e^{2\eta},$$

we still obtain the Robertson–Walker line element (1.3). It can also be shown[8] that (1.1) can be transformed directly into (1.6d) by

$$T = T(s), \quad Y^i = 2x^i/(t + s) \quad (i = 1, 2, 3) \quad (1.7d)$$

provided we choose

$$dT/ds = G(T)/s \quad \text{or} \quad \ln s = \int_0^T dT'/G(T')$$

with $e^\Gamma = G^2/s^2$. In this metric, s corresponds to the age of the universe at time T, $s = 1$ to the singular state $T = 0$ at the beginning. The translation invariance or homogeneity of the world, obscure in the original metric, now appears as the

[4] F. Hoyle, W. A. Fowler, G. R. Burbidge, and E. M. Burbidge, Astrophys. J. 139, 909 (1964).

[5] Y. Ne'eman and G. Tauber, Astrophys. J. (to be published).

[6] L. Infeld and A. Schild, Phys. Rev. 68, 250 (1945).

[7] This definition differs by a factor of 2 from that of Infeld and Schild.[6]

[8] J. W. Weinberg (private communication).

transformation among points of constant age (s = const) and must therefore correspond to the Lorentz transformation by keeping the fictitious point $s = 0$ fixed. The resulting geometry is that of a Lobachevsky space,[9] and the fact that only one function e^{Γ} of one variable s appears makes it mathematically very desirable.

The two forms of the line element (1.6a) and (1.6d) (both are conformal to the flat Minkowski space corresponding to positive or negative curvature, respectively) now form the basis for further calculations. Due to their different structure, they have to be considered separately.[10] In Sec. II, we obtain solutions of the field equations based on (1.6d), while in Sec. III this is done for (1.6a).

II. THE OPEN UNIVERSE ($k = -1$)

Let us now consider the line element given by

$$ds^2 = e^{\Gamma(s)}\epsilon_{\mu\nu}\,dx^\mu\,dx^\nu \tag{2.1}$$

corresponding to the transformation (1.7d). A simple calculation gives for the Christoffel symbols

$$\Gamma^\gamma_{\alpha\beta} = \tfrac{1}{2}\Gamma'(\delta^\gamma_\beta s_\alpha + \delta^\gamma_\alpha s_\beta - \epsilon_{\alpha\beta}s^\gamma) \tag{2.2}$$

and the Einstein tensor

$$G_{\mu\nu} = R_{\mu\nu} - \tfrac{1}{2}g_{\mu\nu}R,$$

$$G_{\mu\nu} = s_\mu s_\nu[\Gamma'' - (\Gamma'/s) - \tfrac{1}{2}\Gamma'^2] - \epsilon_{\mu\nu}[\Gamma'' + (2\Gamma'/s) + \tfrac{1}{4}\Gamma'^2], \tag{2.3}$$

where we have introduced the vector $s^\mu = x^\mu/s$ and its covariant form $s_\mu = \epsilon_{\mu\nu}x^\nu/s$, which is not a true vector, since raising and lowering is performed via the ϵ's rather than the g's. Primes denote differentiation with respect to s.

The function $\Gamma(s)$ is determined by the field equations. For a distribution of matter characterized by a matter density $\rho = T^4_4$ and a pressure $3p = -T^i_i$ in the original coordinate system (1.2), we obtain an energy–momentum tensor with components

$$T_{ij} = \delta_{ij}p[G^2/(1 - \tfrac{1}{4}Y^2)^2], \qquad T_{i4} = 0, \qquad T_{44} = \rho. \tag{2.4}$$

The transformation (1.7d) then leads to

$$T_{\mu\nu} = s_\mu s_\nu e^\Gamma(\rho + p) - \epsilon_{\mu\nu}pe^\Gamma \tag{2.5}$$

in the new coordinates.

The energy–momentum tensor must also satisfy the conservation laws

$$\mathfrak{T}^\nu_{\mu,\nu} - \tfrac{1}{2}\mathfrak{T}^{\alpha\beta}(\partial g_{\alpha\beta}/\partial x^\mu) = 0,$$

where, as usual, German letters denote tensor densities. From the definition of s_μ and s^μ, we find

$$s_\mu s^\mu = 1, \qquad s_\mu = \partial s/\partial x^\mu,$$

and

$$s_{\mu,\nu} = \frac{1}{s}(\epsilon_{\mu\nu} - s_\mu s_\nu), \qquad s^\nu_{,\nu} = 3/s, \qquad s^\nu s_{\mu,\nu} = 0,$$

so that we finally obtain

$$\rho' + (\rho + p)[\tfrac{3}{2}\Gamma' + (3/s)] = 0 \tag{2.6}$$

for the conservation law. If the field equations $G_{\mu\nu} = -\kappa T_{\mu\nu}$ are satisfied, then, of course, (2.6) follows from the Bianchi identities. The field equations yield

$$-\kappa(\rho + p) = e^{-\Gamma}[\Gamma'' - (\Gamma'/s) - \tfrac{1}{2}\Gamma'^2] \tag{2.7a}$$

and

$$-\kappa p = e^{-\Gamma}[\Gamma'' + (2\Gamma'/s) + \tfrac{1}{4}\Gamma'^2] \tag{2.7b}$$

upon equating terms proportional to $\epsilon_{\mu\nu}$ and $s_\mu s_\nu$. These are two equations for the three unknowns Γ, p, and ρ. We therefore still need an additional information which is provided by the equation of state connecting p and ρ. We consider the general class of equations of the form

$$p = a\rho, \tag{2.8}$$

where a is a constant and $c = 1$ in our units.

Upon inserting (2.8) into (2.7) we find upon integrating

$$e^\Gamma = A^2(K - 1/s^{3a+1})^{4/(3a+1)}. \tag{2.9}$$

Since we require that $G = 0$ if $s = 1$, we must take $K = 1$ with A the age constant. For the Hubble factor, we have

$$H = \frac{1}{G}\frac{dG}{dT} = \left(\frac{\Gamma'}{2} + \frac{1}{s}\right)e^{-\frac{1}{2}\Gamma} = \frac{1}{A}\frac{s(s^{3a+1} + 1)}{(s^{3a+1} - 1)^{3(a+1)/3a+1)}}. \tag{2.10}$$

Finally, from (2.7), we obtain for the density

$$\kappa\rho = (12a/A^2)s^{3(a+1)}(s^{3a+1} - 1)^{-6(a+1)/(3a+1)} \quad (a \neq 0), \tag{2.11a}$$

while in the special case $p = 0$ direct calculation gives

$$\kappa\rho = (12/A^2)[s^3/(s - 1)^6] \qquad (a = 0). \tag{2.11b}$$

[9] V. Fock, *The Theory of Space-Time and Gravitation* (Pergamon Press, Inc., New York, 1964).

[10] Both line elements, of course, can be considered simultaneously by replacing s by is. However, in this case we loose the advantage of limiting ourselves to a function of one variable.

Thus, all physical quantities are algebraic functions of s. In Figs. 1 and 2 they are shown for the cases, $a = 0$, $\frac{1}{3}$, and 1, which are of special interest. The transformation to the Robertson–Walker line element is more complicated and requires the evaluation of the time $T = T(s)$, and depends on the value of a. For example, for $a = 0$ and $\frac{1}{3}$, we find

$$T = A[(s^2 - 1)/s - 2 \ln s] \qquad (a = 0),$$

$$T = A[s + (1/s) - 2] \qquad (a = \tfrac{1}{3}),$$

where the constant of integration has been chosen so as to make $T = 0$ if $s = 1$.

III. THE CLOSED UNIVERSE ($k = +1$)

In the case of the closed universe, it is not possible to write the gravitational potentials as a function of one variable, but a considerable simplification is possible by introducing two variables

$$w = 1 - \tfrac{1}{4}s^2 \quad \text{and} \quad v = t/w \qquad (3.1)$$

in terms of which $F(s, t)$ of (1.6a) becomes

$$F(s, t) = f(v)/w^2,$$

with $f(v)$ as yet an arbitrary function of v. From the definition (3.1), it follows that

$$w_\alpha = -\tfrac{1}{2}ss_\alpha = -\tfrac{1}{2}\epsilon_{\alpha\beta}x^\beta, \qquad w^\alpha = -\tfrac{1}{2}x^\alpha,$$

$$v_\alpha = (1/w)[\epsilon_{\alpha 4} - vw_\alpha], \qquad v^\alpha = (1/w)[\epsilon^{\alpha 4} - vw^\alpha].$$

Also

$$\begin{aligned} w_\alpha w^\alpha &= \tfrac{1}{4}s^2 = 1 - w, \\ w_\alpha v^\alpha &= w^\alpha v_\alpha = -(v/w)(2 - w), \\ v_\alpha v^\alpha &= (1 + v^2)/w^2. \end{aligned} \qquad (3.2)$$

The Christoffel symbols are then given by

$$\Gamma^\lambda_{\mu\nu} = \tfrac{1}{2}\Psi' \Lambda^\lambda_{\mu\nu} - (1/w)\Sigma^\lambda_{\mu\nu}, \qquad (3.3)$$

where we have defined

$$\begin{aligned} \Lambda^\lambda_{\mu\nu} &= \delta^\lambda_\mu v_\nu + \delta^\lambda_\nu v_\mu - \epsilon_{\mu\nu}v^\lambda, \\ \Sigma^\lambda_{\mu\nu} &= \delta^\lambda_\mu w_\nu + \delta^\lambda_\nu w_\mu - \epsilon_{\mu\nu}w^\lambda, \\ \Psi &= \ln f. \end{aligned}$$

A straightforward calculation then gives, for the Einstein tensor,

$$\begin{aligned} G_{\mu\nu} &= v_\mu v_\nu(\Psi'' - \tfrac{1}{2}\Psi'^2) \\ &\quad - (\epsilon_{\mu\nu}/w^2)[(\Psi'' + \tfrac{1}{4}\Psi'^2)(1 + v^2) + 3(\Psi' v + 1)], \end{aligned} \qquad (3.4)$$

where primes denote differentiation with respect to v.

We now have to transform the energy–momentum tensor from the original line element (1.1) to the final line element (1.5) with the help of the transformations (1.7a). We start again with the usual form, a pressure given by $3p = -T^i_i$ and a density $\rho = T^4_4$ which gives rise to the components

$$T^{ij} = \delta^{ij}pG^{-2}(1 + \tfrac{1}{4}Y^2)^2, \qquad T^{44} = \rho \qquad (3.5)$$

(where we have taken $k = 1$ for the closed universe).

By the series of transformations

$$\begin{aligned} Y^1 &= R \sin\theta \cos\phi, \\ Y^2 &= R \sin\theta \sin\phi, \\ Y^3 &= R \cos\theta, \end{aligned}$$

and

$$\sin\chi = Y/(1 + \tfrac{1}{4}Y^2), \qquad \tau = \int dT/R,$$

we transform (1.2) into (1.3) and, at the same time, $T^{\mu\nu}$ into

$$\begin{aligned} T^{11} &= p/R^2, \qquad T^{22} = p/R^2 \sin^2\chi, \\ T^{33} &= p/R^2 \sin^2\chi \sin^2\theta, \qquad T^{44} = \rho/R^2. \end{aligned} \qquad (3.6)$$

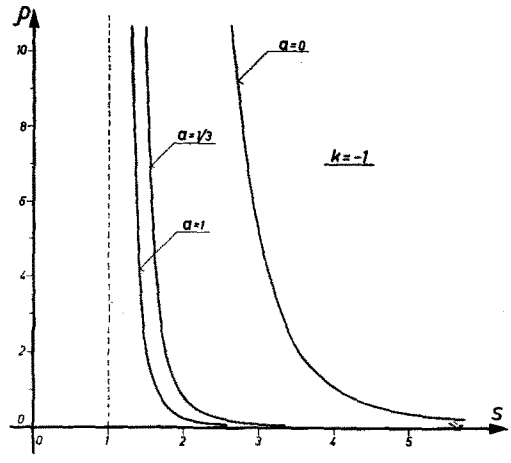

FIG. 1. Density distribution for the open universe.

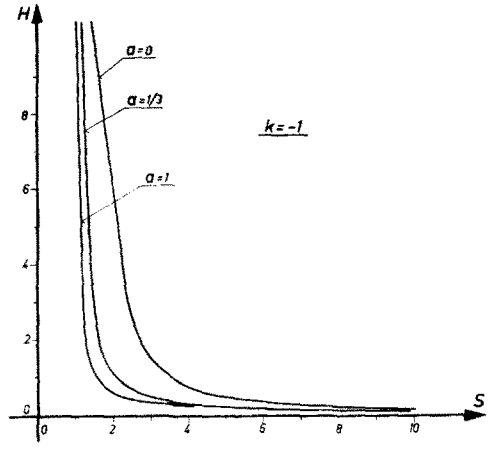

FIG. 2. Hubble factor for the open universe.

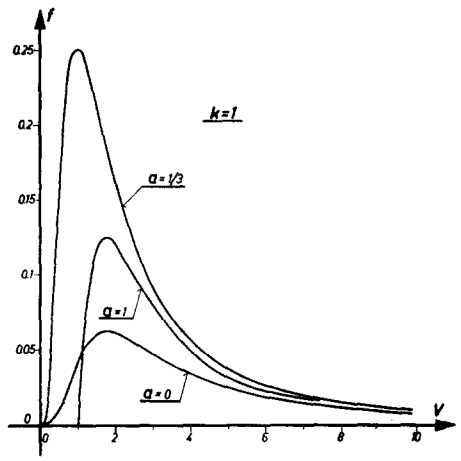

FIG. 3. Solutions of field equations for the closed universe.

Following this with (1.7a) and returning to Cartesian coordinates gives, for the energy–momentum tensor,

$$T^{\mu\nu} = F^{-1}[(p + \rho)(v^\mu v^\nu/v_\alpha v^\alpha) - p\epsilon^{\mu\nu}]. \tag{3.7}$$

Comparison with (3.4) shows that the w dependence drops out by using (3.2), so that (3.7) can be written as

$$T_{\mu\nu} = f(v)\{(p + \rho)[v_\mu v_\nu/(1 + v^2)] - (p/w^2)\epsilon_{\mu\nu}\}. \tag{3.8}$$

Upon equating terms proportional to $v_\mu v_\nu$ and $\epsilon_{\mu\nu}$ in the field equations, we finally obtain

$$(1 + v^2)(\Psi'' - \tfrac{1}{2}\Psi'^2) = -\kappa e^\Psi(p + \rho),$$

$$(1 + v^2)(\Psi'' + \tfrac{1}{4}\Psi'^2) + 3(\Psi' v + 1) = -\kappa e^\Psi p. \tag{3.9}$$

The conservation laws lead to

$$\rho' + \tfrac{3}{2}(p + \rho)[\Psi' + 2v/(1 + v^2)] = 0, \tag{3.10}$$

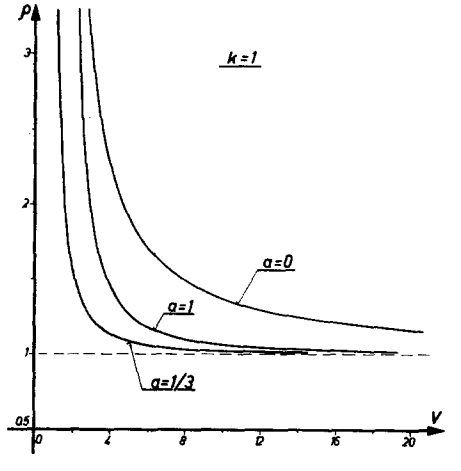

FIG. 4. Density distribution for the closed universe.

where we have used the identities

$$w^\alpha_{,\alpha} = -2, \qquad v^\alpha_{,\alpha} = (v/w^2)(2 + w),$$

$$v_{\alpha,\beta} = \tfrac{1}{2}(v/w)\epsilon_{\alpha\beta} - (v_\alpha w_\beta + w_\alpha v_\beta)/w,$$

$$w_{\alpha,\beta} = -\tfrac{1}{2}\epsilon_{\alpha\beta}.$$

The system of equations (3.9) are again two equations for the three unknowns p, ρ, and Ψ, and have therefore to be augmented again by an equation of state, which we take of the form (2.8).

Upon eliminating p and ρ between the two equations, we obtain

$$(1 + v^2)u'' + 3(1 + a)[u'v + \tfrac{1}{4}(1 + 3a)u] = 0, \tag{3.11}$$

where we have defined the variable u through

$$f(v) = e^\Psi = (\text{const})u^{4/(1+3a)}.$$

In the special case $p = 0$ ($a = 0$), further transformation

$$v = \sinh\theta$$

leads to the solution

$$u = \cosh(\tfrac{1}{2}\theta)\,\operatorname{sech}\theta, \tag{3.12}$$

while from (3.10) we find, for the density,

$$\rho = \rho_0[\cosh\theta/(1 + \cosh\theta)]^3. \tag{3.12a}$$

In the general case, the solution of (3.11) can be expressed as a hypergeometric function

$$u = F[\tfrac{1}{2}c, \tfrac{1}{2}(c - 1); c; z], \tag{3.13}$$

where

$$z = 1 + v^2 \quad \text{and} \quad c = \tfrac{3}{2}(1 + a).$$

For those values of particular interest, such as $a = 1$, $\frac{1}{3}$ (corresponding to $c = 3, 2$), the solutions become degenerate and can be expressed in terms of simple algebraic functions.[11] Thus, for $a = 1$, we find

$$f = u = A[(z - 2)/z^2], \tag{3.14}$$

while the density is given by

$$\rho = \rho_0[z/(z - 2)]^3. \tag{3.14a}$$

Similarily, for $a = \frac{1}{3}$ we obtain

$$f = u^2 = A[(z - 1)/z^2] \tag{3.15}$$

together with

$$\rho = \rho_0[z/(z - 1)]^2. \tag{3.15a}$$

[11] Of the two possible solutions, we have chosen the one which seems to give the correct physical behavior at large values of v.

The behavior of these solutions and the corresponding density distribution as a function of v are shown in Figs. 3 and 4.

Finally, upon performing the transformation (1.7a), these solutions can be expressed in terms of the original coordinates if so desired. It is not difficult to see that, as a result of (1.7a),

$$\tan \tau = v$$

and thus

$$R^2 = (1 + v^2)f(v) = zf(v), \tag{3.16}$$

where $f(v)$ is determined by the field equations. Also, the age T is given by

$$T = \int R(\tau)\, d\tau = \frac{1}{2}\int Rz^{-1}(z-1)^{-\frac{1}{2}}\, dz, \tag{3.17}$$

which gives, for the Hubble factor,

$$H = \frac{1}{R}\frac{dR}{dT} = -2z(z-1)^{\frac{1}{2}}\frac{d}{dz}\left(\frac{1}{R}\right). \tag{3.18}$$

In Fig. 5 the Hubble factor H is shown for $a = 0$, $\frac{1}{3}$, and 1.

We therefore have a comparatively simple method of obtaining all solutions of the cosmological problem[12] for an equation of state of the form (2.8). For other equations of state, the results are more complicated, though they still provide some simplification on account of the conformal nature of the line element.

IV. GENERALIZATIONS

If, in addition to the gravitational field, other fields are present, their effect must also be taken into account either as additional contributions. or as the source of the pressure and density distribution. In the first case, we obtain the effect of the gravitational field on their distributions, while in the second case they provide the missing equation of state. We have considered the fields corresponding to a scalar meson, an electromagnetic field, and a second-rank tensor for both cases with results to be reported elsewhere.[13]

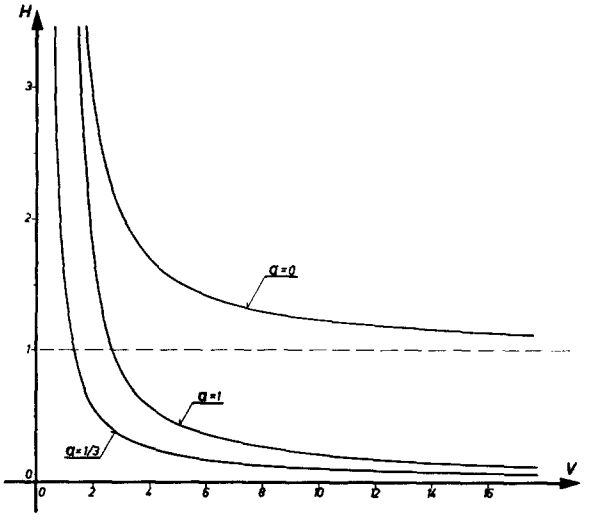

FIG. 5. Hubble factor for the closed universe.

Another possible extension consists in considering line elements which, although conformally flat, contain more general functions than the ones required by homogeneity and isotropy. In this way, it might be possible to describe universes which are not homogeneous. Work along these lines is in progress and promises to give interesting results.

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[12] We have limited ourselves to the case of vanishing cosmological constant. However, it is quite simple to generalize our results also for nonvanishing cosmological constant by introducing a term proportional to F into the field equations.

[13] Cf. G. Tauber, Tensor 14, 18 (1963).

One-Dimensional Ising Model with General Spin

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The one-dimensional Ising model with general spin S has been formulated as an eigenvalue problem of order $2S + 1$. Two methods to reduce the order to $[S + 1]$ have been developed for calculating the energy and the susceptibility at zero external field. Exact solutions for $S = \frac{3}{2}$ and $S = 1$ have been obtained. Numerical calculations of $S = \frac{3}{2}$, 1, and $\frac{1}{2}$ have been compared.

I. INTRODUCTION

THE one-dimensional Ising model with spin $\frac{1}{2}$ was solved by Ising[1] using a combinatorial method, and by Kramers and Wannier[2] and Kubo[3] using a matrix method. The one-dimensional Ising model with higher spin S can also be transformed into an eigenvalue problem whose order is $2S + 1$. In this paper two methods for reducing the order of the problem to $[S + 1]$ are developed. Here $[S + 1]$ denotes the greatest integer not exceeding $S + 1$. We first develop a perturbation method employed previously[4] in a treatment of the dilute Ising model, and then demonstrate an implicit differentiation method.

By these means we calculate the energy, specific heat, and susceptibility in zero external field. For $S = \frac{3}{2}$ we calculate these quantities exactly and explicitly; for $S = 1$ the thermodynamic quantities are transcribed from the previous results[4] for the idealized annealed case of the dilute Ising model of $S = \frac{1}{2}$. The results are compared with those of $S = \frac{1}{2}$.

II. EIGENVALUE PROBLEM

Consider a crystal lattice with an Ising spin of spin S at each lattice site, labeled $i = 1, 2, \cdots N$. The total energy of this system is given by

$$H = -2J \sum_i S_i S_{i+1} - g\mu\mathfrak{H} \sum_i S_i, \qquad (2.1)$$

where S_i is the z component of the spin operator ($S_i = S, S - 1, \cdots -S$), J measures the magnitude of the exchange interaction, and g and μ denote gyromagnetic ratio and Bohr magneton. $J > 0$ corresponds to ferromagnetic interaction and $J < 0$ antiferromagnetic interaction.

In the case of a one-dimensional system with cyclic boundary conditions, the partition function Z is expressed as the trace of a matrix:

$$Z = \mathrm{Tr}\ V_{\mathfrak{H}}^N, \qquad (2.2)$$

$$V_{\mathfrak{H}} = V_2^{\frac{1}{2}} V_1 V_2^{\frac{1}{2}}, \qquad (2.3)$$

where

$$\langle S' |\ V_1\ | S'' \rangle = \exp\,(2JS'S''/kT), \qquad (2.4)$$

$$\langle S' |\ V_2\ | S'' \rangle = \delta_{S'S''} \exp\,(g\mu\mathfrak{H}S'/kT). \qquad (2.5)$$

Hereafter the case $S = \frac{3}{2}$ is treated as an example. Then

$$V_1 = \begin{bmatrix} e^{9K} & e^{3K} & e^{-3K} & e^{-9K} \\ e^{3K} & e^{K} & e^{-K} & e^{-3K} \\ e^{-3K} & e^{-K} & e^{K} & e^{3K} \\ e^{-9K} & e^{-3K} & e^{3K} & e^{9K} \end{bmatrix}, \qquad (2.6)$$

$$V_2 = \begin{bmatrix} e^{3L} & & & \\ & e^{L} & & \\ & & e^{-L} & \\ & & & e^{-3L} \end{bmatrix}, \qquad (2.7)$$

$$V_2^{\frac{1}{2}} V_1 V_2^{\frac{1}{2}} = \begin{bmatrix} e^{9K+3L} & e^{3K+2L} & e^{-3K+L} & e^{-9K} \\ e^{3K+2L} & e^{K+L} & e^{-K} & e^{-3K-L} \\ e^{-3K+L} & e^{-K} & e^{K-L} & e^{3K-2L} \\ e^{-9K} & e^{-3K-L} & e^{3K-2L} & e^{9K-3L} \end{bmatrix}, \qquad (2.8)$$

[1] E. Ising, Z. Physik 31, 253 (1925).
[2] H. A. Kramers and G. H. Wannier, Phys. Rev. 60, 252, 263 (1941).
[3] R. Kubo, Busseiron-Kenkyu (in Japanese) No. 1, 1 (1943).
[4] S. Katsura and B. Tsujiyama, in *Proceedings of the Conference on Phenomena in the Neighborhood of Critical Points* (National Bureau of Standards, Washington, D. C., 1965), p. 219.

where

$$K = J/2kT, \qquad L = g\mu\mathfrak{H}/2kT.$$

In the limit of an infinitely large crystal, the partition function per lattice site is given by

$$\lim_{N\to\infty} Z^{1/N} = \lambda_m, \tag{2.9}$$

where λ_m is the largest eigenvalue of the matrix (2.8).

III. PERTURBATION METHOD

Since we are interested mainly in the energy and the susceptibility at zero field, it is sufficient to derive λ_m exactly only up to second order in powers of L. $V_{\mathfrak{H}}$ is expressed as a sum of two parts which are an even function of the external field L and an odd function of it:

$$V_{\mathfrak{H}} = \begin{bmatrix} A & C & D & B \\ C & E & F & D \\ D & F & E & C \\ B & D & C & A \end{bmatrix} + \begin{bmatrix} D' & A' & B' & 0 \\ A' & C' & 0 & -B' \\ B' & 0 & -C' & -A' \\ 0 & -B' & -A' & D' \end{bmatrix}, \tag{3.1}$$

where

$$\begin{aligned} A &= k^{18}\cosh 3L, & A' &= k^{6}\sinh 2L, \\ B &= k^{-18}, & B' &= k^{-6}\sinh L, \\ C &= k^{6}\cosh 2L, & C' &= k^{2}\sinh L, \\ D &= k^{-6}\cosh L, & D' &= k^{18}\sinh 3L, \\ E &= k^{2}\cosh L, & e^{K} &= k^{2}. \\ F &= k^{-2}, \end{aligned} \tag{3.2}$$

By applying a similarity transformation T_1,

$$T_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & & & 1 \\ & 1 & 1 & \\ & 1 & -1 & \\ 1 & & & -1 \end{bmatrix} = T_1^{-1}, \tag{3.3}$$

we have

$$T_1^{-1} V_{\mathfrak{H}} T_1 = \begin{bmatrix} A+B & C+D & & \\ C+D & E+F & & \\ & & E-F & C-D \\ & & C-D & A-B \end{bmatrix} + \begin{bmatrix} & & A'-B' & D' \\ & & C' & A'+B' \\ A'-B' & C' & & \\ D' & A'+B' & & \end{bmatrix}. \tag{3.4}$$

Next, a second transformation T_2

$$T_2 = \begin{bmatrix} \sin\theta & \cos\theta & & \\ \cos\theta & -\sin\theta & & \\ & & \sin\varphi & \cos\varphi \\ & & \cos\varphi & -\sin\varphi \end{bmatrix} = T_2^{-1}, \tag{3.5}$$

is applied to (3.4) in such a way that the first matrix becomes diagonal by choosing proper values of θ and φ. That is,

$$\tan 2\theta = 2(C+D)/(E+F-A-B), \tag{3.6}$$

$$\tan 2\varphi = 2(C-D)/(A-B-E+F). \tag{3.6'}$$

When θ is restricted such that $0 < \theta < \frac{1}{2}\pi$,

$$\begin{aligned} \sin\theta &= [\tfrac{1}{2}(1 \mp (1+\tan^2 2\theta)^{-\frac{1}{2}}]^{\frac{1}{2}}, \\ \cos\theta &= [\tfrac{1}{2}(1 \pm (1+\tan^2 2\theta)^{-\frac{1}{2}}]^{\frac{1}{2}}, \end{aligned} \tag{3.7}$$

where the upper sign is taken when $0 < \theta < \frac{1}{4}\pi$, and the lower sign when $\frac{1}{4}\pi < \theta < \frac{1}{2}\pi$. Similar restrictions apply to φ.

Then

$$T_2^{-1}T_1^{-1}V_{\mathfrak{H}}T_1T_2 = \begin{bmatrix} H_1^{(0)} & & & \\ & H_2^{(0)} & & \\ & & H_3^{(0)} & \\ & & & H_4^{(0)} \end{bmatrix} + \begin{bmatrix} & & H_{13}^{(1)} & H_{14}^{(1)} \\ & & H_{23}^{(1)} & H_{24}^{(1)} \\ H_{31}^{(1)} & H_{32}^{(1)} & & \\ H_{41}^{(1)} & H_{42}^{(1)} & & \end{bmatrix}, \tag{3.8}$$

where

$$\begin{aligned} H_1^{(0)} &= \tfrac{1}{2}\{(A+B+E+F) \\ &\quad \pm [(E+F-A-B)^2 + 4(C+D)^2]^{\frac{1}{2}}\}, \\ H_2^{(0)} &= \tfrac{1}{2}\{(A+B+E+F) \\ &\quad \mp [(E+F-A-B)^2 + 4(C+D)^2]^{\frac{1}{2}}\}, \\ H_3^{(0)} &= \tfrac{1}{2}\{(E-F+A-B) \\ &\quad \pm [(E-F-A+B)^2 + 4(C-D)^2]^{\frac{1}{2}}\}, \\ H_4^{(0)} &= \tfrac{1}{2}\{(E-F+A-B) \\ &\quad \mp [(E-F-A+B)^2 + 4(C-D)^2]^{\frac{1}{2}}\}. \end{aligned} \tag{3.9}$$

When $C + D > 0$, the upper signs of $H_1^{(0)}$ and $H_2^{(0)}$ are taken, and when $C + D < 0$, the lower signs. When $C - D > 0$, the upper signs of $H_3^{(0)}$ and $H_4^{(0)}$ are taken, and when $C - D < 0$, the lower signs. (In $H_1^{(0)}$ and $H_2^{(0)}$, $C + D$ is always positive and $H_1^{(0)}$ is largest.) Expressions for $H_{ij}^{(1)}$ are omitted.

In order to obtain λ_m in the case of $L \simeq 0$, $H^{(0)}$ is regarded as the unperturbed term and $H^{(1)}$ as the perturbation. From second-order perturbation theory (first-order perturbation term vanishes)

$$\lambda_m = H_1^{(0)} + \frac{H_{13}^{(1)}H_{31}^{(1)}}{H_1^{(0)} - H_3^{(0)}} + \frac{H_{14}^{(1)}H_{41}^{(1)}}{H_1^{(0)} - H_4^{(0)}}. \tag{3.10}$$

Terms of $O(L^2)$ do not appear from the third- and higher-order terms in the perturbation.

Here we derive λ_m up to $O(L^2)$.

$$H_1^{(0)} = \lambda_{00} + L^2\lambda_{01} + O(L^4), \tag{3.11}$$

$$\begin{aligned} H_{13}^{(1)}H_{31}^{(1)}/(H_1^{(0)} - H_3^{(0)}) &= L^2\lambda_{13} + O(L^4), \\ H_{14}^{(1)}H_{41}^{(1)}/(H_1^{(0)} - H_4^{(0)}) &= L^2\lambda_{14} + O(L^4), \end{aligned} \tag{3.12}$$

then

$$\lambda_{00} = \tfrac{1}{2}(k^{18} + k^2 + k^{-18} + k^{-2}) + \tfrac{1}{2}l^{\frac{1}{2}} \tag{3.13}$$

$$= \cosh 9K + \cosh K + [(\cosh 9K - \cosh K)^2 + 4\cosh^2 3K]^{\frac{1}{2}}, \tag{3.14}$$

$$\lambda_{01} = \tfrac{1}{4}(9k^{18} + k^2) + \tfrac{1}{4}[(k^{18} + k^{-18} - k^2 - k^{-2}) \times (9k^{18} - k^2) + 4(k^6 + k^{-6})(4k^6 + k^{-6})]/l^{\frac{1}{2}}, \tag{3.15}$$

$$\lambda_{13} + \lambda_{14} = [2r(p^2 + q^2) + t]/(4r^2 - m)l^{\frac{1}{2}}, \tag{3.16}$$

where

$$\begin{aligned} l &= \eta^2 + 4(k^6 + k^{-6})^2, \\ \eta &= k^{18} + k^{-18} - k^2 - k^{-2}, \\ m &= v^2 + 4(k^6 - k^{-6})^2, \\ v &= -k^{18} + k^{-18} + k^2 - k^{-2}, \\ r &= k^{-18} + k^{-2} + \tfrac{1}{2}l^{\frac{1}{2}}, \\ p &= (2k^6 - k^{-6})(l^{\frac{1}{2}} + \eta)^{\frac{1}{2}} + k^2(l^{\frac{1}{2}} - \eta)^{\frac{1}{2}}, \\ q &= 3k^{18}(l^{\frac{1}{2}} + \eta)^{\frac{1}{2}} + (2k^6 + k^{-6})(l^{\frac{1}{2}} - \eta)^{\frac{1}{2}}, \\ t &= v(p^2 - q^2) + 4pq(k^6 - k^{-6}). \end{aligned} \tag{3.17}$$

The energy E at zero field is given by

$$\begin{aligned} \frac{E}{NJ} &= -\frac{1}{2}\left(\frac{1}{\lambda_{00}}\right)\left(\frac{\partial\lambda_{00}}{\partial K}\right) \\ &= -\frac{1}{4}\frac{1}{\lambda_{00}}\Big\{9e^{9K} - 9e^{-9K} + e^K - e^{-K} \\ &\quad + \frac{(e^{9K} + e^{-9K} - e^K - e^{-K})(9e^{9K} - 9e^{-9K} - e^K + e^{-K}) + 12(e^{6K} - e^{-6K})}{[(e^{9K} + e^{-9K} - e^K - e^{-K})^2 + 4(e^{3K} + e^{-3K})^2]^{\frac{1}{2}}}\Big\}. \end{aligned} \tag{3.18}$$

The expression for the specific heat is omitted here. The zero field susceptibility χ is given by

$$\frac{kT\chi}{N(g\mu)^2} = \frac{1}{4}\frac{\partial^2 \ln\lambda}{\partial L^2}\bigg|_{L=0} = \frac{\lambda_{01} + \lambda_{13} + \lambda_{14}}{2\lambda_{00}}. \tag{3.19}$$

Substituting (3.13), (3.15), and (3.16) into (3.19), χ can be expressed as a function of reduced temperature K. In the final expression, double roots disappear and square roots appear only in $l^{\frac{1}{2}}$.

IV. ALTERNATIVE DERIVATION OF THE ZERO-FIELD SUSCEPTIBILITY

In general the zero-field susceptibility χ can also be obtained in the following way. When $\beta(\mathfrak{IC})$ is chosen as an arbitrary even function of $\mathfrak{IC}$,

$$\begin{aligned} M &= kT\frac{\partial}{\partial\mathfrak{IC}}\log\lambda_m(\beta(\mathfrak{IC})) \\ &= kT\frac{1}{\lambda_m}\frac{\partial\beta}{\partial\mathfrak{IC}}\frac{\partial\lambda_m}{\partial\beta}, \end{aligned} \tag{4.1}$$

$$\chi = \left(\frac{\partial M}{\partial\mathfrak{IC}}\right)_{\mathfrak{IC}=0} = kT\frac{1}{\lambda_m}\left(\frac{\partial^2\beta}{\partial\mathfrak{IC}^2}\right)_{\mathfrak{IC}=0}\left(\frac{\partial\lambda_m}{\partial\beta}\right)_{\mathfrak{IC}=0}. \tag{4.2}$$

When

$$\det(V_{\mathfrak{IC}} - \lambda\cdot 1) = f(\lambda, \beta(\mathfrak{IC})) \tag{4.3}$$

is known, it gives

$$\chi = -kT\frac{1}{\lambda_m}\left(\frac{\partial^2\beta}{\partial\mathfrak{IC}^2}\right)\frac{\partial f(\lambda_m, \beta)/\partial\beta}{\partial f(\lambda_m, \beta)/\partial\lambda_m}. \tag{4.2'}$$

Hereafter we put

$$a = e^{-K} = e^{-J/2kT}, \qquad b = e^{-L}, \tag{4.4}$$

$$\beta = b + \frac{1}{b} = 2\cosh(g\mu/2kT)\mathfrak{IC} = 2\cosh L.$$

This method does not require knowledge of $\lambda_m(\mathfrak{IC})$ but only of $\lambda_m(0)$ and of $f(\lambda_m, \beta(\mathfrak{IC}))$.

From the first term of (3.4) together with $L = 0$,

$$\det(V_0 - \lambda\cdot 1) = f(\lambda, \beta(0)) = g_1(\lambda)g_2(\lambda), \tag{4.5}$$

$$g_1(\lambda) = \lambda^2 - \lambda(a + a^{-1} + a^9 + a^{-9}) + (a + a^{-1})(a^9 + a^{-9}) - (a^3 + a^{-3})^2,$$
$$g_2(\lambda) = \lambda^2 + \lambda(a - a^{-1} + a^9 - a^{-9}) + (a - a^{-1})(a^9 - a^{-9}) - (a^3 - a^{-3})^2. \quad (4.5')$$

Hence

$$f(0, \beta(0)) = 2[\cosh 20K - 3\cosh 16K + \cosh 12K + 4\cosh 8K - 2\cosh 4K - 1]. \quad (4.6)$$

Now

$$\frac{\partial f(\lambda, \beta(\mathfrak{IC}))}{\partial \lambda} = -\sum_{i=1}^{4} f_i(\lambda, b) = -\sum_{i=1}^{2}\left[f_i(\lambda, b) + f_i\left(\lambda, \frac{1}{b}\right)\right], \quad (4.7)$$

where $f_i(\lambda, b)$ is a minor determinant of $V_{\mathfrak{IC}} - 1\cdot\lambda$ excluding the ith row and ith column:

$$f_1(\lambda, b) = \begin{vmatrix} a^{-1}b^{-1} - \lambda & a & a^3b \\ a & a^{-1}b - \lambda & a^{-3}b^2 \\ a^3b & a^{-3}b^2 & a^{-9}b^3 - \lambda \end{vmatrix}$$
$$= -\lambda^3 + \lambda^2[a^{-1}(b + b^{-1}) + a^{-9}b^3] - \lambda(a^{-10}b^4 + a^{-2} + a^{-10}b^2 - a^6b^2 - a^{-6}b^4 - a^2) + (a^{-11}b^3 + 2ab^3 - a^5b^3 - 2a^{-7}b^3), \quad (4.8)$$

and

$$f_2(\lambda, b) = \begin{vmatrix} a^{-9}b^{-3} - \lambda & a^3b^{-1} & a^9 \\ a^3b^{-1} & a^{-1}b - \lambda & a^{-3}b^2 \\ a^9 & a^{-3}b^2 & a^{-9}b^3 - \lambda \end{vmatrix}$$
$$= -\lambda^3 + \lambda^2[a^{-9}(b^3 + b^{-3}) + a^{-1}b] - \lambda(a^{-10}b^4 + a^{-10}b^{-2} + a^{-18} - a^{18} - a^{-6}b^4 - a^6b^{-2}) + (a^{-19}b + 2a^9b - a^{17}b - a^{-15}b - a^{-3}b). \quad (4.9)$$

Hence

$$-\frac{\partial f(\lambda, \beta(\mathfrak{IC}))}{\partial \lambda} = -4\lambda^3 + 3\lambda^2\{a^{-1}(b + b^{-1}) + a^{-9}(b^3 + b^{-3})\} - 2\lambda\{a^{-10}(b^4 + b^{-4}) + a^{-10}(b^2 + b^{-2}) - a^{-6}(b^4 + b^{-4}) - a^6(b^2 + b^{-2}) + (a^{-2} - a^2) + (a^{-18} - a^{18})\} + (b^3 + b^{-3})(a^{-11} - 2a^{-7} + 2a - a^5) + (b + b^{-1})(a^{-19} - a^{-15} - a^{-3} + 2a^9 - a^{17}). \quad (4.10)$$

Integrating (4.10) and using (4.6), we have

$$f(\lambda, \beta(\mathfrak{IC})) = \lambda^4 - 2\lambda^3(a^{-1}\cosh L + a^{-9}\cosh 3L) + 2\lambda^2\{(a^{-10} - a^{-6})\cosh 4L + (a^{-10} - a^6)\cosh 2L + \tfrac{1}{2}(a^{-2} - a^2) + \tfrac{1}{2}(a^{-18} - a^{18})\} - 2\lambda\{a^{-11} - 2a^{-7} + 2a - a^5)\cosh 3L + (a^{-19} - a^{-15} - a^{-3} + 2a^9 - a^{17})\cosh L\} + 2[\cosh 20K - 3\cosh 16K + \cosh 12K + 4\cosh 3K - 2\cosh 4K - 1]. \quad (4.11)$$

Hence

$$\frac{\partial}{\partial\beta} f(\lambda, \beta)\Big|_{\mathfrak{IC}=0} = -\lambda^3(a^{-1} + 9a^{-9}) + \lambda^2(20a^{-10} - 16a^{-6} - 4a^6) - \lambda\{9(a^{-11} - 2a^{-7} + 2a - a^5) + (a^{-19} - a^{-15} - a^{-3} + 2a^9 - a^{17})\}. \quad (4.12)$$

From (4.5)

$$\partial f(\lambda, \beta(0))/\partial\lambda|_{\lambda_m} = g_1'(\lambda_m)g_2(\lambda_m) + g_1(\lambda_m)g_2'(\lambda_m) = g_1'(\lambda_m)g_2(\lambda_m) = l^{\frac{1}{2}}[2\lambda_m(a + a^9) + 4 - 2(a^8 + a^{-8})]. \quad (4.13)$$

Thus the zero-field susceptibility is given by

$$kT\chi/N(g\mu)^2 = \tfrac{1}{2}[\lambda_m^2(a^{-1} + 9a^{-9}) + 4\lambda_m(a^6 + 4a^{-6} - 5a^{-10}) + 9(a^{-11} - 2a^{-7} + 2a - a^5) + a^{-19} - a^{-15} - a^{-3} + 2a^9 - a^{17}][f'(\lambda_m, \beta(0))]^{-1}, \quad (4.14)$$

where $f'(\lambda_m, \beta(0))$ is given by (4.13) and λ_m, the largest eigenvalue in case of no external field, is given by (3.14).

V. ISING MODEL WITH $S = 1$

The results of the previous paper[4] for the case of the annealed dilute Ising model with $S = \frac{1}{2}$ can be transcribed for those of the Ising model with $S = 1$ by modifying minor notations. Substitution of $J \to 4J$, $K \to 4K$, $d = 1$, and $m = g\mu$ in the results of the previous paper give immediately the partition function, the energy, and the susceptibility at zero magnetic field of the model $S = 1$.

Partition function:

$$\lambda_m = \tfrac{1}{2}\{2\cosh 4K + 1 + [(2\cosh 4K - 1)^2 + 8]^{\frac{1}{2}}\}. \quad (5.1)$$

The energy:

$$\frac{E}{NJ} = -\frac{1+a}{1-a}\left\{1 + \frac{a-5+a^{-1}}{[(a+a^{-1}-1)^2+8]^{\frac{1}{2}}}\right\}, \tag{5.2}$$

where $a = e^{-4K} = e^{-2J/kT}$. [Symbol a in this section is different from that in Sec. IV.]

The susceptibility:

$$\frac{kT\chi}{N(g\mu)^2} = \frac{1}{a+a^{-1}+1+[(a+a^{-1}-1)^2+8]^{\frac{1}{2}}}\left(\frac{a^{-2}-a^{-1}+3}{[(a+a^{-1}-1)^2+8]^{\frac{1}{2}}} + a^{-1}\right.$$
$$\left. + \left\{4a^{-2}+2+\frac{4\{(a+a^{-1}-1)(a^{-2}-\frac{1}{2})+4a^{-1}\}}{[(a+a^{-1}-1)^2+8]^{\frac{1}{2}}}\right\}\{3a-a^{-1}+1+[(a+a^{-1}-1)^2+8]^{\frac{1}{2}}\}^{-1}\right). \tag{5.3}$$

The method of Sec. IV can also be applied and gives

$$\frac{kT\chi}{2N(g\mu)^2} = \frac{1}{a}\frac{\lambda_m + a - 1}{3\lambda_m^2 - 2(1+2a^{-1})\lambda_m + (a^{-2}+2a^{-1}-a^2-2)}. \tag{5.3'}$$

Both expressions (5.3) and (5.3') are transformed into a simple form:

$$\frac{kT\chi}{2(g\mu)^2N} = \frac{1}{4a^2(a+2)} \times \left\{1 + \frac{4a^3+5a^2-a+1}{a[(a+a^{-1}-1)^2+8]^{\frac{1}{2}}}\right\}. \tag{5.4}$$

In this case the largest eigenvalue λ_m as a function of finite magnetic field[5] can be obtained easily.

$$\lambda_m = 2.3^{-\frac{1}{2}}[\nu(L,K)]^{\frac{1}{2}} \times \cos\left(\tfrac{1}{3}\arccos\{\tfrac{1}{2}(3^{\frac{3}{2}})\kappa(L,K)[\nu(L,K)]^{-\frac{3}{2}}\}\right) + \tfrac{1}{3}[e^{4K}(L^2+L^{-2})+1], \tag{5.5}$$

where

$$\nu(L,K) = \tfrac{1}{3}e^{8K}(L^4+L^{-4}) + (1-\tfrac{1}{3}e^{4K})(L^2+L^{-2}) - \tfrac{1}{3}e^{8K} + \tfrac{1}{3} + e^{-8K}, \tag{5.6}$$

$$\kappa(L,K) = \tfrac{2}{27}e^{12K}(L^6+L^{-6}) + (-\tfrac{1}{9}e^{8K}+\tfrac{1}{3}e^{4K})(L^4+L^{-4}) + (-\tfrac{1}{9}e^{12K}-\tfrac{1}{9}e^{4K}+\tfrac{1}{3}e^{-4K}+\tfrac{1}{3})(L^2+L^{-2}) + \tfrac{4}{9}e^{8K} - \tfrac{4}{3}e^{4K} + \tfrac{2}{27} + 2e^{-4K} - \tfrac{2}{3}e^{-8K}. \tag{5.7}$$

[5] When we regard λ_m as a complex function of a complex fugacity variable $z = e^L$, the singularities in the complex z plane are determined by the zeros of $\nu(L,K) = 0$ and $27\kappa^2(L,K) - 4\kappa^3(L,K) = 0$. The complex values of L for a given K which satisfies the above equations are neither real nor pure imaginary. $\nu(L,K)$ and $\kappa(L,K)$ are both symmetric with respect to L and L^{-1}. This implies that λ_m has nonreal singularities inside the circle $|z| = 1$. The one of which the absolute value is the smallest determines the radius of convergence of the fugacity series. The model is an example in which the radius of convergence and the singularities have no connection with the fugacity at the phase transition. [cf. S. Katsura and H. Fujita, J. Chem. Phys. **19**, 795 (1951); Progr. Theoret. Phys. (Kyoto) **6**, 498 (1951); S. Katsura, Advan. Phys. **12**, 391 (1963); J. L. Lebowitz and O. Penrose, J. Math. Phys. **5**, 841 (1964).

Here we used Slater's formula[6] to diagonalize a symmetric matrix of the third order.

VI. HIGH-TEMPERATURE AND LOW-TEMPERATURE EXPANSIONS

High-temperature expansion of the energy and the susceptibility with general spin S can be calculated straightforwardly.[7] The results are

$$\lambda_m = (2S+1) \times [1 + \tfrac{2}{9}S^2(S+1)^2(J/kT)^2 + \cdots], \tag{6.1}$$

$$E/NJ = -\tfrac{4}{9}S^2(S+1)^2(J/kT) + \cdots, \tag{6.2}$$

$$\chi kT/N(g\mu)^2 = \tfrac{1}{3}S(S+1)[1 + \tfrac{4}{3}S(S+1)(J/kT) + \cdots]. \tag{6.3}$$

For low temperature we have the following asymptotic formula from the results in previous sections.

$S = 1$:

$$\lambda_m \sim \exp(2J/kT) + 3\exp(-2J/kT) + \cdots, \tag{6.4}$$

$$\chi kT/N(g\mu)^2 \sim \tfrac{1}{2}\exp(4J/kT) + \cdots, \tag{6.5}$$

$S = \frac{3}{2}$:

$$\lambda_m \sim \exp(9J/2kT) + \exp(-3J/2kT) + 3\exp(-9J/2kT) + \cdots, \tag{6.6}$$

$$\chi kT/N(g\mu)^2 \sim \tfrac{3}{4}\exp(9J/kT) + \cdots. \tag{6.7}$$

[6] J. C. Slater, *Quantum Mechanics of Atomic Structure* (McGraw-Hill Book Company, Inc., New York, 1960), Vol. 1, Appendix 3.

[7] G. S. Rushbooke and D. J. Morgan, Mol. Phys. **4**, 291 (1961).

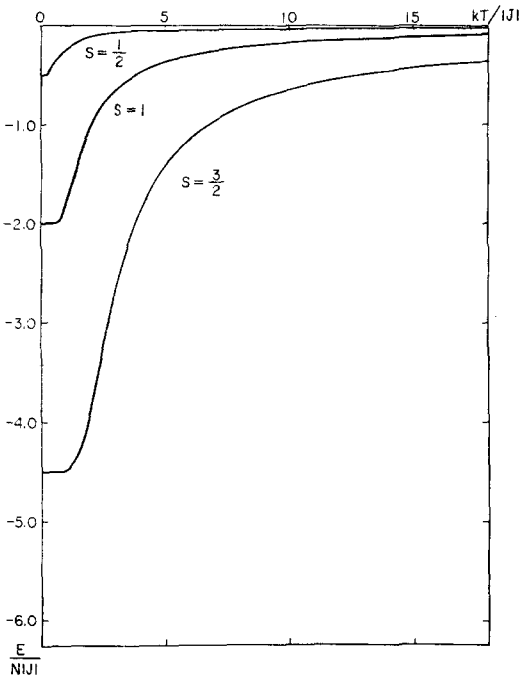

FIG. 1. Energy. The ordinate and the abscissa denote $E/N\,|J|$ and $kT/|J|$, respectively.

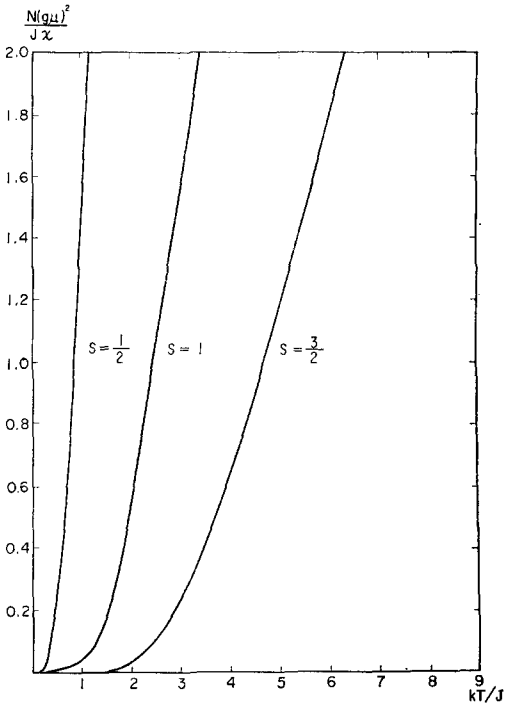

FIG. 3. Inverse susceptibility for ferromagnetic interaction. The ordinate and the abscissa denote $N(g\mu)^2/J\chi$ and kT/J, respectively.

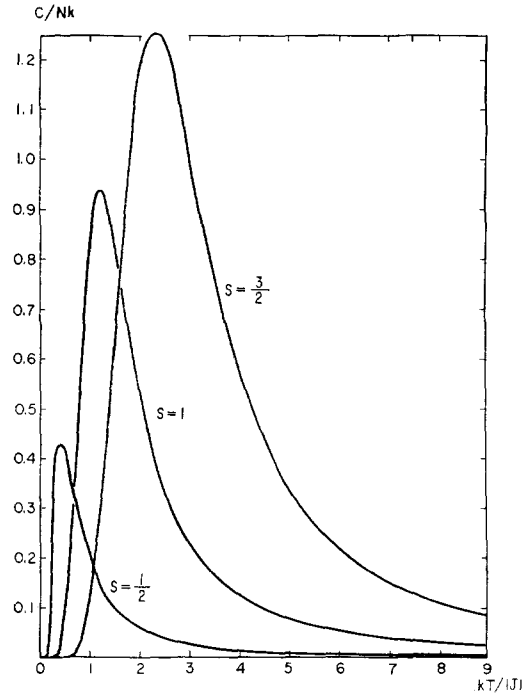

FIG. 2. Specific heat. The ordinate and the abscissa denote C/Nk and $kT/|J|$, respectively.

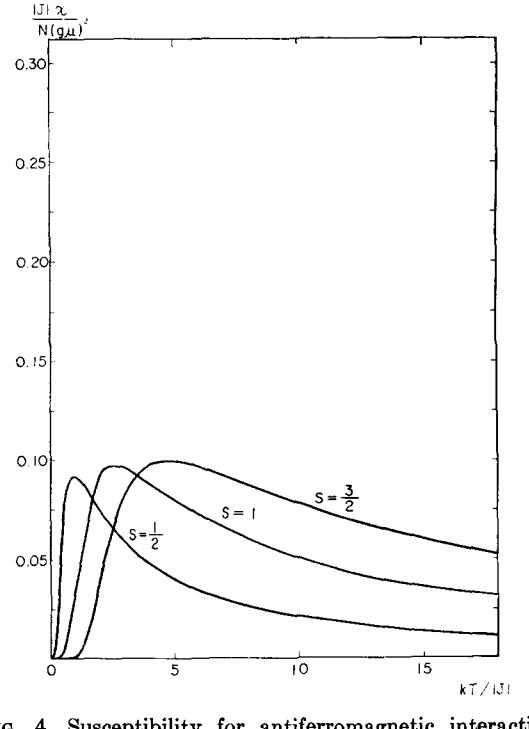

FIG. 4. Susceptibility for antiferromagnetic interaction. The ordinate and the abscissa denote $|J|\,\chi/N(g\mu)^2$ and $kT/|J|$, respectively.

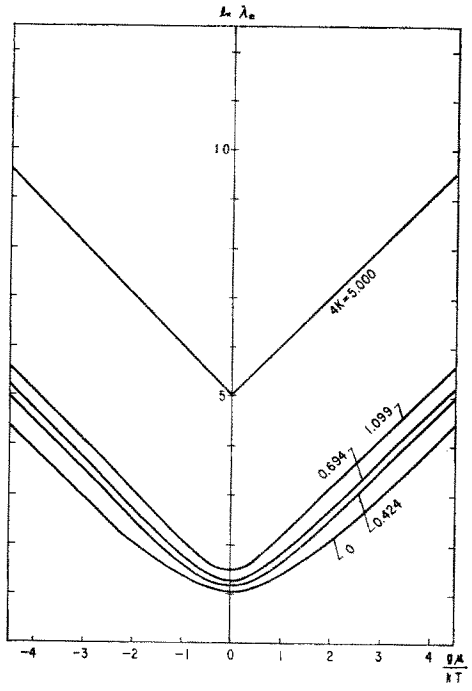

FIG. 5. The largest eigenvalue λ_m of $S = 1$ as a function of the magnetic field and the temperature for ferromagnetic interaction $J > 0$. The ordinate denotes ln λ_m. Parameters denote $4K = 2J/kT$.

These results together with those of $S = \frac{1}{2}$ can be written as

$$\lambda_m \sim \exp(2S^2J/kT) + \cdots, \tag{6.8}$$

$$\chi kT/N(g\mu)^2 \sim \tfrac{1}{2}S \exp 4S^2J/kT + \cdots. \tag{6.9}$$

These expansions were used to check the results of the previous sections numerically.

VII. NUMERICAL RESULTS

The energy, specific heat, and susceptibility of the one-dimensional Ising model with $S = \frac{3}{2}$ and $S = 1$ have been calculated. The agreement of the susceptibility between both methods, (3.19) and (4.14), has been confirmed numerically.

Now we compare the numerical results of three cases, $S = \frac{1}{2}$, 1, and $\frac{3}{2}$. Figure 1 shows the energy of these cases in zero magnetic field. Figure 2 shows the specific heat. The energy and the specific heat is the same for ferro- and antiferromagnetic interaction. Figure 3 shows the inverse susceptibility for ferromagnetic interaction. Figure 4 shows the susceptibility for antiferromagnetic interaction. Figure 5 shows λ_m for $S = 1$ as a function of the magnetic field and temperature for ferromagnetic interaction.

Both methods can be applied to the problem of general spin, and the eigenvalue problem of order $2S + 1$ can be reduced to order $[S + 1]$. The problems of $S = 2$ and $\frac{5}{2}$ can be reduced to an algebraic equation of the third order, and those of $S = 3$ and $\frac{7}{2}$ of the fourth order.

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Canonical Root Vectors of SU_n*

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The present paper extends the study of SU_n to the determination of particular root vectors and fundamental weights. The root vectors are chosen so as to show explicitly the canonical nesting of subgroups $SU_n \supset SU_{n-1} \times U_1$, $SU_{n-1} \supset SU_{n-2} \times U_1$, etc. Explicit matrix representations of the fundamental representations are given. The results are all dependent upon the use of n vectors which define the fundamental region of SU_n. Eigenvalues of fundamental invariant operators are also given in terms of these n vectors.

INTRODUCTION

It has been shown by Cartan[1] that the root vectors and fundamental weights of SU_n may be expressed in terms of n $(n-1)$-component vectors ω_i $i = 1, 2, \cdots, n$. These vectors have apparently not been further exploited, though they appear as the coefficients $\lambda_i^{(j)}$ in Ref. 2. The present paper leans heavily upon the use of these vectors and their use provides insight into the structure of SU_n.

In Sec. I, we find the vectors ω_i which show explicitly the nesting of subgroups $SU_n \supset SU_{n-1} \times U_1$, $SU_{n-1} \supset SU_{n-2} \times U_1$, etc., and the properties of these vectors are discussed. In Sec. II, the results of Cartan,[1] with regard to the fundamental weights of SU_n, are given and the labeling of irreducible representations of SU_n is reviewed.

Section III contains simple matrix representations of the fundamental representations, and Sec. IV deals with the symmetric coupling coefficients in terms of the ω_i and the eigenvalues of the invariant operators of SU_n.

I.

The generators of SU_n are H_i $i = 1, 2, \cdots, l$, and E_{ij} $i, j = 1, \cdots, n$ $i \neq j$, where $l = n - 1$ is the rank of the group. The labeling $E_\alpha \equiv E_{ij}$ is sometimes used and then, $-\alpha = (ji)$ if $\alpha = (ij)$. The canonical commutation relations are

$$\begin{aligned} [H_i, H_j] &= 0, \\ [H_i, E_{jk}] &= (2n)^{-\frac{1}{2}}(\omega_i^{(i)} - \omega_k^{(i)})E_{jk} \end{aligned} \tag{1.1}$$

or

$$\begin{aligned} [H, E_{jk}] &= (2n)^{-\frac{1}{2}}(\omega_j - \omega_k)E_{jk}, \\ [E_{ij}, E_{ji}] &= (2n)^{-\frac{1}{2}}(\omega_i - \omega_j)\cdot H, \\ [E_{ij}, E_{rs}] &= (2n)^{-\frac{1}{2}}(\delta_{jr} E_{is} - \delta_{is} E_{rj}), \end{aligned}$$

where $\omega_i^{(j)}$ is the ith component of the jth vector, $i = 1, \cdots, l$ and $j = 1, \cdots, n$.

The n l-component vectors ω_i are not orthogonal, but form the same angle with respect to each other.

$$\omega_i \cdot \omega_j = \delta_{ij} - (1/n) \tag{1.2}$$

or

$$|\omega_i| = |l/n|^{\frac{1}{2}} \tag{1.3}$$

and $\cos\theta = -1/l$, where θ is the angle between two different vectors.

The ω_i are not linearly independent and one relationship exists between them, namely,

$$\sum_{i=1}^{n} \omega_i = 0. \tag{1.4}$$

The normalization (1.3) is such that the group metric g_{AB}, $A, B, = i, \alpha$ (i.e., A and B range over the entire algebra) assumes the form $g_{AB} = \delta_{A,-B}$ where $-A = A$ for $A = i$ and $-A = (ji)$ if $A = (ij)$.

Consequently the ω_i satisfy

$$\sum_{r=1}^{n} \omega_r^{(i)} \omega_r^{(j)} = \delta^{ij}. \tag{1.5}$$

Two root vectors $\omega_i - \omega_j$ and $\omega_r - \omega_s$ form an angle ϕ given by

$$\frac{(\omega_i - \omega_j)\cdot(\omega_r - \omega_s)}{|\omega_i - \omega_j|\,|\omega_r - \omega_s|} = \tfrac{1}{2}(\delta_{ir} + \delta_{js} - \delta_{is} - \delta_{jr})$$

or

$$\begin{aligned} \cos\phi &= 0 \\ &= \pm 1 \\ &= \pm\tfrac{1}{2}, \end{aligned}$$

which identifies the group as SU_n.

The ω_i vectors point from the origin to n points of an l-dimensional space. These points are the vertices of the fundamental region of the root space. The root vectors are the edges of the fundamental regions.

For $l = 1, 2, 3$, the fundamental region is a line, an equilateral triangle, a tetrahedran, etc.

* This work was partially supported by the National Science Foundation.

† Submitted in partial fulfillment of the requirements of the degree of Doctor of Philosophy, University of California, Los Angeles, California.

[1] E. Cartan, Ann. Mat. 4, 209 (1927); Bull. Soc. Math. France 41, 53 (1913).

[2] L. C. Biedenharn, J. Math. Phys. 4, 436 (1963).

TABLE I. Components of the ω_i vectors.

	$\times 2^{-\frac{1}{2}}$	$\times 6^{-\frac{1}{2}}$	$\times 12^{-\frac{1}{2}}$	$\times 20^{-\frac{1}{2}}$	$\cdots \times [(l-1)l]^{-\frac{1}{2}}$	$\times [l(l+1)]^{-\frac{1}{2}}$
$u_1=\omega_1=$	1	1	1	1	1	1
$u_n=\omega_2=$	−1	1	1	1	1	1
$u_{n-1}=\omega_3=$	0	−2	1	1	1	1
$u_{n-2}=\omega_4=$	0	0	−3	1	1	1
$u_3=\omega_l=$	0	0	0	0	$-l+1$	1
$u_2=\omega_n=$	0	0	0	0	0	$-l$

The fundamental region may be oriented arbitrarily with respect to a Cartesian coordinate system. If the coordinate axes are labeled by the H_i and an orientation of the fundamental region is specified, then the vectors ω_i, and consequently the root vectors, are determined. As an example consider the group SU_4 with the tetrahedran as fundamental region. The tetrahedran may be oriented such that one of its four triangular faces lies in the 1–2 plane. The edges of the face are the root vectors for SU_3. The tetrahedran may also be oriented such that one of the three edges of the above-mentioned triangular face lies in the 1 direction. This edge of the triangular face gives the root vectors for SU_2.

The orientation specified above displays the decomposition

$$SU_4 \supset SU_3 \times H_3,$$
$$SU_3 \supset SU_2 \times H_2,$$

where H_2 and H_3 are independently the generators for the group U_1.

It is clear that an orientation of the fundamental region of SU_n exists which displays the decomposition

$$SU_n \supset SU_{n-1} \times H_l,$$
$$SU_{n-1} \supset SU_{n-2} \times H_{l-1}, \quad \text{etc.}$$

The above-described canonical orientation of the fundamental region is ensured if the ω_i are chosen as follows. Place ω_n along the $(-l)$ direction. Place ω_{n-1} along the $(-l+1)$ direction and in the l, $l-1$ subspace. Place ω_{n-2} along the $(-l+2)$ direction and in the l, $l-1$, $l-2$ subspace, etc. ω_1 is determined from (1.4).

Two features of this recipe reflect choices which prove convenient. First is the labeling of the vectors, which is such that the operators of SU_{n-1} are

$$E'_{ij} = (n)^{\frac{1}{2}}(n-1)^{-\frac{1}{2}}E_{ij}, \quad i,j = 1,2,\cdots,l,$$
$$H'_i = (n)^{\frac{1}{2}}(n-1)^{-\frac{1}{2}}H_i, \quad i = 1,\cdots,l-1, \tag{1.6}$$

and the operators of SU_{n-2} are

$$E''_{ij} = (n)^{\frac{1}{2}}(n-2)^{-\frac{1}{2}}E_{ij}, \quad i,j = 1,2,\cdots,l-1,$$
$$H''_i = (n)^{\frac{1}{2}}(n-2)^{-\frac{1}{2}}H_i, \quad i = 1,2,\cdots,l-2, \tag{1.7}$$

etc. Second is the choice of ω_n along $(-l)$ instead of the (l) direction. This has the effect of making $\omega_1 > \omega_i$ the value of which becomes apparent later.

The components $\omega_i^{(j)}$ are given by

$$\omega_i^{(j)} = [j(j+1)]^{-\frac{1}{2}}\theta(j-i+1)[1-i\delta_{i-1,i}] \tag{1.8}$$

and explicitly in Table I.

Here $\theta(x)$ has the properties

$$\theta(x) = 1, \quad x \geq 0,$$
$$\theta(x) = 0, \quad x < 0. \tag{1.9}$$

II.

In discussing the weights, it is convenient to introduce another set of n u vectors related to the ω vectors in the following way.

$$u_1 = \omega_1, \quad u_2 = \omega_n, \quad u_3 = \omega_{n-1}, \quad u_n = \omega_2. \tag{2.1}$$

This is simply a relabeling of the n vectors with the virtue that

$$u_i > u_{i+1} \qquad i = 1,2,\cdots,l. \tag{2.2}$$

The ordering of two vectors, say u_1 and u_2, according to $u_1 > u_2$ means that the first nonvanishing component of the vector $u_1 - u_2$, reading the components from left to right, is positive. If the first nonvanishing component is negative, then $u_1 < u_2$.

Now, the l fundamental weights (that is, the l highest weights of the l fundamental representations) may be easily expressed in terms of the u vectors. Let π_i be the highest weight of the ith fundamental representation. Then[1]

$$\pi_i = (2n)^{-\frac{1}{2}}\sum_{j=1}^{i} u_j, \qquad i = 1,2,\cdots,l \tag{2.3}$$

and the l fundamental weights are ordered by

$$\pi_i > \pi_{i+1}, \qquad i = 1,2,\cdots,l-1. \tag{2.4}$$

The root vectors r_{ij}

$$r_{ij} = (2n)^{-\frac{1}{2}}(u_i - u_j) \tag{2.5}$$

are ordered as follows:

$$\begin{aligned} r_{ik} &> r_{jk}, \qquad i < j, \\ r_{ij} &> r_{ji}, \qquad i < j. \end{aligned} \tag{2.6}$$

The l simple roots r_i are thus given by

$$r_i = r_{i,i+1} = (2n)^{-\frac{1}{2}}(u_i - u_{i+1}), \tag{2.7}$$

and the $\frac{1}{2}l(l+1)$ plus roots are given by

$$r^+_{ij} = r_{ij} = (2n)^{-\frac{1}{2}}(u_i - u_j), \qquad i < j. \tag{2.8}$$

The highest weight M of an irreducible representation is given by

$$M = \sum_{i=1}^{l} \lambda_i \pi_i. \tag{2.9}$$

The l numbers λ_i may be used to characterize an irreducible representation. M may also be expressed in terms of the u_i to give

$$M = (2n)^{-\frac{1}{2}} \sum_{i=1}^{l} \eta_i u_i, \tag{2.10}$$

where

$$\eta_i = \sum_{j=1}^{n-i} \lambda_j. \tag{2.11}$$

The l numbers η_i may also be used to characterize an irreducible representation and in fact they are the lengths of the rows of the Young tableaux associated with the representation, whereas the λ_i are the overlaps of one row over the next.

Let the highest state of the irreducible representation labeled by the set of η_i be given by $|\uparrow\{\eta\}\rangle$; then

$$H\,|\uparrow\{\eta\}\rangle = (2n)^{-\frac{1}{2}} \sum_{i=1}^{l} \eta_i u_i\,|\uparrow\{\eta\}\rangle,$$

and from (1.2) we have

$$(2n)^{\frac{1}{2}}(u_i - u_n)\cdot H\,|\uparrow\{\eta\}\rangle = \eta_i\,|\uparrow\{\eta\}\rangle; \tag{2.12}$$

that is, the l operators $(2n)^{\frac{1}{2}}(u_i - u_n)\cdot H$ when applied to the highest state give the l η_i.

III.

The matrix representations of the generators corresponding to the first fundamental representation are given below

$$\begin{aligned} h^{[1]} &= (2n)^{-\frac{1}{2}} \sum_{i=1}^{n} u_i\,|i\rangle\langle i|, \\ \epsilon^{[1]}_{ij} &= (2n)^{-\frac{1}{2}}\,|i\rangle\langle j|, \end{aligned} \tag{3.1}$$

where $|i\rangle\langle j|$ is a matrix with 1 in the ith row, jth column and zero elsewhere.

The representation (3.1) of the first fundamental representation is well known. Representations of the other fundamental representations are given below.

Second representation:

$$\begin{aligned} h^{[2]} &= (2n)^{-\frac{1}{2}} \sum_{(ij)} (u_i + u_j)\,|(ij)\rangle\langle(ij)|, \\ \epsilon^{[2]}_{pq} &= (2n)^{-\frac{1}{2}} \sum_{\substack{r\neq p \\ r\neq q}} \epsilon\binom{pq}{r}\,|(pr)\rangle\langle(qr)|, \end{aligned} \tag{3.2}$$

where (ij) is a particular combination with no repetitions of two of the integers 1, 2, $\cdots$, n and the sum is over the combinations.

The numbers $\epsilon\binom{pq}{r}$ have the following properties:

$$\begin{aligned} &\epsilon\binom{pq}{r} = \epsilon\binom{qp}{r} = \pm 1, \\ &\epsilon\binom{pq}{r}\epsilon\binom{qm}{r}\epsilon\binom{pm}{r} = 1, \\ &\epsilon\binom{pq}{r}\epsilon\binom{pr}{q}\epsilon\binom{rq}{p} = -1. \end{aligned} \tag{3.3}$$

A particular solution is

$$\epsilon\binom{pq}{r} = \phi(p - r)\phi(q - r), \tag{3.4}$$

where

$$\begin{aligned} \phi(x) &= 1, \quad \text{if} \quad x > 0, \\ \phi(x) &= -1, \quad \text{if} \quad x < 0. \end{aligned} \tag{3.5}$$

Third representation:

$$\begin{aligned} h^{[3]} &= (2n)^{-\frac{1}{2}} \sum_{(ijk)} (u_i + u_j + u_k)\,|(ijk)\rangle\langle(ijk)|, \\ \epsilon^{[3]}_{pq} &= (2n)^{-\frac{1}{2}} \sum_{\substack{(rs)\neq p \\ \neq q}} \epsilon\binom{pq}{rs}\,|(prs)\rangle\langle(qrs)|\}, \end{aligned} \tag{3.6}$$

where (ijk) is a particular combination with no repetitions of three of the integers 1, 2, $\cdots$, n.

The numbers $\epsilon\binom{pq}{rs}$ satisfy

$$\begin{aligned} &\epsilon\binom{pq}{rs} = \epsilon\binom{pq}{sr} = \epsilon\binom{qp}{rs} = \epsilon\binom{qp}{sr} = \pm 1, \\ &\epsilon\binom{pq}{rs}\epsilon\binom{pm}{rs}\epsilon\binom{mq}{rs} = 1, \\ &\epsilon\binom{pq}{rs}\epsilon\binom{ps}{rq}\epsilon\binom{qs}{rp} = -1. \end{aligned} \tag{3.7}$$

A particular solution is

$$\epsilon\binom{pq}{rs} = \phi(p - r)\phi(p - s)\phi(q - r)\phi(q - s). \tag{3.8}$$

The above may be generalized to the other fundamental representations.

IV.

The anticommutation relations of (3.1) define the symmetric coupling coefficients

$$\begin{aligned}
\{h^{[1]}, \epsilon_{ij}^{[1]}\} &= (2n)^{-\frac{1}{2}}(u_i + u_j)\epsilon_{ij}^{[1]}, \\
\{\epsilon_{ij}^{[1]}, \epsilon_{ji}^{[1]}\} &= (1/n^2)1 + (2n)^{-\frac{1}{2}}(u_i + u_j)\cdot h^{[1]}, \\
\{\epsilon_{ij}^{[1]}, \epsilon_{rs}^{[1]}\} &= (2n)^{-\frac{1}{2}}(\delta_{jr}\,\epsilon_{is}^{[1]} + \delta_{is}\,\epsilon_{rj}^{[1]}), \\
\{h_i^{[1]}\ h_j^{[1]}\} &= (1/n^2)\,\delta_{ij}\,1 + 2(2n)^{-\frac{1}{2}} \\
&\quad \times \sum_{k=1}^{l}\left(\sum_{r=1}^{n} u_r^{(i)}u_r^{(j)}u_r^{(k)}\right)h_k^{[1]}.
\end{aligned} \tag{4.1}$$

Thus, the symmetric coupling coefficients $[_{AB}{}^{C}]$ in the relation

$$\{l_A^{[1]}, l_B^{[1]}\} = [_{AB}{}^{C}]l_C^{[1]}, \tag{4.2}$$

where $l_A^{[1]}$ runs over the whole algebra, are given by

$$\begin{aligned}
[ijk] &= 2(2n)^{-\frac{1}{2}}\sum_{r=1}^{n} u_r^{(i)}u_r^{(j)}u_r^{(k)}, \\
[i(jk)(kj)] &= (2n)^{-\frac{1}{2}}(u_i^{(i)} + u_k^{(i)}), \\
[\alpha\beta\gamma] &= (2n)^{-\frac{1}{2}};\ \text{ here } r_\alpha + r_\beta + r_\gamma = 0, \\
[(jk)(kj)i] &= (2n)^{-\frac{1}{2}}(u_i^{(i)} + u_k^{(i)}),
\end{aligned} \tag{4.3}$$

where g^{AB} has been used to lower $[_{AB}{}^{C}]$ to $[_{ABC}]$.

Biedenharn[2] has constructed l invariant operators using the symmetric coupling coefficients. They are

$$\begin{aligned}
I_2 &= g^{AB}L_AL_B, \\
I_3 &= g^{AB}L_A[_B{}^{CD}]L_CL_D, \\
I_4 &= g^{AB}L_A[_B{}^{CD}][_D{}^{EF}]L_CL_EL_F, \\
&\vdots \\
I_n &= g^{AB}L_A[\ ]\cdots[\ ]\underbrace{LL\cdots L}_{n-1\text{ factors}}.
\end{aligned} \tag{4.4}$$

The eigenvalues of these operators are[3]

$$\begin{aligned}
\tilde{I}_2 &= (M + 2R)_iM_i, \\
\tilde{I}_3 &= (M + 2R)_iA_{ij}M_j, \\
\tilde{I}_4 &= (M + 2R)_iA_{ij}A_{jk}M_k, \\
&\vdots \\
\tilde{I}_n &= (M + 2R)_i\underbrace{A_{ij}\cdots A_{lm}}_{n-2\text{ factors}}M_m,
\end{aligned} \tag{4.5}$$

where

$$A_{ij} = [ijk]M_k + \sum_{+\alpha} s_\alpha^{(i)}r_\alpha^{(j)}, \tag{4.6}$$

$$s_\alpha^{(i)} = (2n)^{-\frac{1}{2}}(u_i^{(i)} + u_k^{(i)}), \qquad \alpha = (jk), \tag{4.7}$$

and

$$R_i = \tfrac{1}{2}\sum_{+\alpha} r_\alpha^{(i)} = \sum_{j=1}^{l}\pi_j^{(i)}. \tag{4.8}$$

R is seen to be a highest weight where $\lambda_i = 1$, $i = 1, \cdots, l$. Now

$$\begin{aligned}
[ijk]R_k &= (2n)^{-1}\sum_{k=1}^{l}\sum_{r=1}^{n}\sum_{s<t}^{n} u_r^{(i)}u_r^{(j)}u_r^{(k)}(u_s^{(k)} - u_t^{(k)}) \\
&= \sum_{+\alpha} s_\alpha^{(i)}r_\alpha^{(j)} - X_{ij},
\end{aligned} \tag{4.9}$$

where

$$X_{ij} = (2n)^{-1}\sum_{s<t}(u_t^{(i)}u_s^{(j)} - u_s^{(i)}u_t^{(j)}). \tag{4.10}$$

So,

$$\sum_{+\alpha} s_\alpha^{(i)}r_\alpha^{(j)} = [ijk]R_k + X_{ij}; \tag{4.11}$$

i.e., $\sum_{+\alpha} s_\alpha^{(i)}r_\alpha^{(j)}$ has been split into its symmetric and antisymmetric parts.

A_{ij} takes the form

$$A_{ij} = [ijk]L_k + X_{ij} \tag{4.12}$$

and $\tilde{I}_r$ is now expressed as

$$\tilde{I}_r = (L + R)_iB_{ij}(L - R)_j, \tag{4.13}$$

where

$$L_i = (M + R)_i \tag{4.14}$$

and

$$B_{ij} = \underbrace{A_{il}A_{lm}\cdots A_{pq}A_{qj}}_{r-2\text{ factors}}. \tag{4.15}$$

The question as to whether or not these invariants suffice to label uniquely the irreducible representations of SU_n was answered by Biedenharn. The argument runs as follows.

The quantities $\tilde{I}_r$, as functions of L_i, are invariant under the Weyl reflection group.[4] That is, when the vector L is reflected in the hyperplanes perpendicular to the root vectors, the $\tilde{I}_r$ are invariant. The Jacobian with respect to L_i of the l independent invariants of this Weyl reflection group factors into $\frac{1}{2}[n(n-1)]$ linear forms, which, when equated to zero, give the reflecting hyperplanes.[5] The factoring of the Jacobian of the $\tilde{I}_r$ is equivalent to the factoring of the Jacobian of l quantities

$$\tilde{K}_r = \sum_{i=1}^{n}(L\cdot u_i)^r, \qquad r = 2, \cdots, n, \tag{4.16}$$

and this Jacobian has the properties of the Jacobian of the l independent invariants of the Weyl reflection group; therefore, the $\tilde{I}_r$ are independent.[2]

[3] M. Micu, Nucl. Phys. **60**, 353 (1964).

[4] G. Racah, CERN Report 61-8 (1961).

[5] C. Chevalley, Am. J. Math. **77**, 778 (1955).

Another set of invariant operators of SU_n are the familiar quantities

$$N_r = \sum_{\substack{all\\ indices}}^{n} \underbrace{E_{ij}E_{jk}\cdots E_{rs}E_{si}}_{r \text{ factors}}, \qquad (4.17)$$

where the summation is now over all i, j, etc., and

$$E_{ij} = u_i \cdot H. \qquad (4.18)$$

The eigenvalues $\tilde{N}_r$ are[6]

$$\tilde{N}_r = \sum_{\substack{all\\ indices}}^{n} [\delta_{ik}u_k\cdot M + W_i\cdot u_k][\delta_{kr}u_r\cdot M + W_k\cdot u_r] \times \underbrace{\cdots [\delta_{ts}\,u_s\cdot M + W_t\cdot u_s]}_{r-1 \text{ factors}}(u_s\cdot M), \qquad (4.19)$$

where

$$W_i = \sum_{i<j} r_{ij} = (2n)^{-\frac{1}{2}}[(n-i)u_i] + \pi_i. \qquad (4.20)$$

This expression may be rearranged to give

$$\tilde{N}_r = \sum_{\substack{all\\ indices}}^{n} \underbrace{C_{ik}C_{kr}\cdots C_{ts}}_{r-1 \text{ factors}}(u_s\cdot M),$$

where

$$C_{ik} = \delta_{ik}\,u_k\cdot L + W_{ik}$$

and

$$W_{ik} = (2n)^{-\frac{1}{2}}[\tfrac{1}{2}(n+1)\,\delta_{ik} - \theta(k-i)].$$

The independence argument given above may be applied to the $\tilde{N}_r$ to establish them as fundamental invariants.

[6] A. M. Perelomov and V. S. Popov, JETP Letters 1, 15 (1965); see also F. Halbwachs, "Invariants Fondamentaux des Groups SU_n et $SU(n,1)$," preprint (1965).

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Representation Functions of the Group of Motions of Clifford Space*

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We find the representation functions of the group of motions of the three-dimensional Clifford space and of the three-dimensional Einstein space. These functions are generalizations of spherical and cylindrical waves of three-dimensional Euclidian space and reduce to these familiar functions in the Euclidian limit. The generalization of the plane wave is also found.

1. INTRODUCTION

PHYSICAL space is often characterized as a three-dimensional metric space of absolute parallelism with positive definite symmetric metric and zero torsion. This space has an associated group of motions, that is, a group of coordinate transformations that leave the metric (and also the connection) invariant. This group is a six-parameter group usually decomposed into three displacements and three rotations.

A generalization of the above space may be made by allowing the torsion to be nonzero, but uniform. This space still has a six-parameter group of motions with transformations corresponding to displacements and rotations. In this paper we find the eigenfunctions of the operators associated with these transformations and show their relationship to the usual eigenfunctions of Euclidian space, i.e., the spherical, cylindrical, and plane waves.

2. SPECIFICATION OF THE SPACE

The generalized space S considered here may be characterized as follows[1,2]:

$$L^{\mu}_{\alpha\beta\gamma}(+) = 0, \qquad (2.1)$$

$$\Omega^{\mu}_{\alpha\beta|\gamma+} = 0, \qquad (2.2)$$

$$g_{\alpha\beta|\gamma+} = 0, \qquad (2.3)$$

where[3] $L^{\mu}_{\alpha\beta\gamma}(+)$, $\Omega^{\mu}_{\alpha\beta}$, and $g_{\alpha\beta}$ are tensors representing the curvature, torsion, and metric. The $|^{+}$ sign appearing above means the covariant derivative with respect to the (+) connection $L^{\mu}_{\alpha\beta} \equiv L^{\mu}_{\alpha\beta}(+)$ and

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[1] L. P. Eisenhart, *Continuous Groups of Transformations* (Dover Publications Inc., New York, 1961), pp. 51 and 231.

[2] E. Cartan and J. A. Schouten, Akad. van Wetens, Amsterdam, Proc. 29, 803 (1926).

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where the summation is now over all i, j, etc., and

$$E_{ij} = u_i \cdot H. \qquad (4.18)$$

The eigenvalues $\tilde{N}_r$ are[6]

$$\tilde{N}_r = \sum_{\substack{all\\ indices}}^{n} [\delta_{ik}u_k\cdot M + W_i\cdot u_k][\delta_{kr}u_r\cdot M + W_k\cdot u_r] \times \underbrace{\cdots [\delta_{ts}\,u_s\cdot M + W_t\cdot u_s]}_{r-1 \text{ factors}}(u_s\cdot M), \qquad (4.19)$$

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$$W_i = \sum_{i<j} r_{ij} = (2n)^{-\frac{1}{2}}[(n-i)u_i] + \pi_i. \qquad (4.20)$$

This expression may be rearranged to give

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the $(-)$ connection $L^{\mu}_{\alpha\beta}(-)$, where

$$L^{\mu}_{\alpha\beta} \equiv L^{\mu}_{\alpha\beta}(+) \equiv \Gamma^{\mu}_{\alpha\beta} + \Omega^{\mu}_{\alpha\beta}, \tag{2.4}$$

$$L^{\mu}_{\alpha\beta}(-) \equiv \Gamma^{\mu}_{\alpha\beta} - \Omega^{\mu}_{\alpha\beta}, \tag{2.5}$$

$\Gamma^{\mu}_{\alpha\beta}$ and $\Omega^{\mu}_{\alpha\beta}$ are, respectively, symmetric and antisymmetric in α and β.

$$\Gamma^{\mu}_{\alpha\beta} = \Gamma^{\mu}_{\beta\alpha}, \tag{2.6}$$

$$\Omega^{\mu}_{\alpha\beta} = -\Omega^{\mu}_{\beta\alpha}. \tag{2.7}$$

Explicitly, the $(\pm)$-covariant derivatives and a sometimes used (0)-covariant derivative are given below where A_{μ} is an arbitrary covariant vector.

$$A_{\mu|\nu+} \equiv \partial_{\nu}A_{\mu} - L^{\sigma}_{\mu\nu}(+)A_{\sigma}, \tag{2.8}$$

$$A_{\mu|\nu-} \equiv \partial_{\nu}A_{\mu} - L^{\sigma}_{\mu\nu}(-)A_{\sigma}, \tag{2.9}$$

$$A_{\mu|\nu 0} \equiv \partial_{\nu}A_{\mu} - \Gamma^{\sigma}_{\mu\nu}A_{\sigma}. \tag{2.10}$$

From (2.3) it follows that $\Omega_{\mu\alpha\beta}$ is completely antisymmetric. If the torsion is taken to be zero, S reduces to the usual Euclidian space.

3. ADDITIONAL PROPERTIES OF S

The properties of the space defined by the $(-)$ connection are the same as the space defined by the $(+)$ connection; that is,

$$L^{\mu}_{\alpha\beta\gamma}(-) = 0 \tag{3.1}$$

and

$$\Omega^{\mu}_{\alpha\beta|\gamma-} = 0. \tag{3.2}$$

Also, the space defined by $g_{\alpha\beta}$ and $\Gamma^{\mu}_{\alpha\beta}$ is an Einstein space, that is,

$$g_{\alpha\beta|\gamma 0} = 0 \tag{3.3}$$

and

$$B_{\alpha\beta} = -2Kg_{\alpha\beta}, \tag{3.4}$$

where $B_{\alpha\beta}$ is the contracted curvature tensor formed from $\Gamma^{\mu}_{\alpha\beta}$. Consequently,

$$\Gamma^{\mu}_{\alpha\beta} = \{{}^{\mu}_{\alpha\beta}\}, \tag{3.5}$$

where $\{{}^{\mu}_{\alpha\beta}\}$ is the Christoffel symbol.

4. ENNUPLE FIELDS

Since S has the property $L^{\mu}_{\alpha\beta\gamma}(\pm) = 0$, the two equations $\lambda_{\mu|\nu\pm} = 0$ may be integrated to give two vector fields which are individually everywhere parallel to themselves.

If we take three vector fields $\lambda^{i}_{\mu}(+)$ which are orthogonal at a point, then they are orthogonal everywhere. We think of these three vector fields as defining a basis at every point of S, the bases at different points being related by $(+)$-parallel transfer.

The same considerations apply to three vector fields orthogonal at a point and satisfying $\lambda^{i}_{\mu|\nu-} = 0$. They are orthogonal everywhere and are related by $(-)$-parallel transfer.

We define an ennuple fundamental, or metric tensor $\bar{g}_{ij}$ by

$$\begin{aligned} \bar{g}_{ij} &= 1 \quad \text{if} \quad i = j, \\ \bar{g}_{ij} &= 0 \quad \text{if} \quad i \neq j, \end{aligned} \tag{4.1}$$

and the ennuple tensor $\bar{g}^{ij}$ by $\bar{g}^{ij}\bar{g}_{jk} = \delta^{i}_{k}$.

We then associate with the vectors λ^{i}_{μ} the vectors

$$\lambda_{i\mu} = \bar{g}_{ij}\lambda^{j}_{\mu}, \tag{4.2}$$

$$\lambda^{i\mu} = g^{\mu\nu}\lambda^{i}_{\nu}, \tag{4.3}$$

and

$$\lambda^{\mu}_{i} = \bar{g}_{ij}g^{\mu\nu}\lambda^{j}_{\nu}. \tag{4.4}$$

5. GROUP OF MOTIONS

Consider the following six quantities:

$$X_{i}(\pm) \equiv \lambda^{\mu}_{i}(\pm)\,\partial_{\mu}. \tag{5.1}$$

Since the $\lambda^{i}_{\mu}(\pm)$ satisfy Killing's equation

$$\lambda^{i}_{\mu|\nu 0} + \lambda^{i}_{\nu|\mu 0} = 0, \tag{5.2}$$

the quantities (5.1) are the generators of coordinate transformations that leave the metric invariant. The commutation relations of these generators are as follows:

$$[X_{i}(+), X_{j}(+)] = C_{ij}{}^{k}(+)X_{k}(+), \tag{5.3a}$$

$$[X_{i}(-), X_{j}(-)] = C_{ij}{}^{k}(-)X_{k}(-), \tag{5.3b}$$

$$[X_{i}(+), X_{j}(-)] = 0, \tag{5.3c}$$

where

$$C_{ij}{}^{k}(\pm) = \pm 2\lambda^{k}_{\mu}(\pm)\lambda^{\alpha}_{i}(\pm)\lambda^{\beta}_{j}(\pm)\Omega^{\mu}_{\alpha\beta}. \tag{5.4}$$

The $C_{ij}{}^{k}(\pm)$ are constant scalars because they satisfy

$$C_{ij}{}^{k}(\pm)_{|\nu\pm} = 0 = \partial_{\nu}\,C_{ij}{}^{k}(\pm). \tag{5.5}$$

They also satisfy the Jacobi relations and are thus generators of a Lie group.

The $C_{ij}{}^{k}(+)$ and $C_{ij}{}^{k}(-)$ are related by choosing the $\lambda^{i}_{\mu}(+)$ and $\lambda^{i}_{\mu}(-)$ to coincide at one point. Then

$$C_{ij}{}^{k}(+) = -C_{ij}{}^{k}(-). \tag{5.6}$$

The quantity

$$C_{ijk}(\pm) = C_{ij}{}^{l}(\pm)\bar{g}_{lk} \tag{5.7}$$

is totally antisymmetric as a result of the antisymmetry of $\Omega_{\alpha\beta\gamma}$. Consequently, we set

$$C_{ij}{}^{k}(+) = 2K^{\frac{1}{2}}\epsilon_{ij}{}^{k}, \tag{5.8a}$$

$$C_{ij}{}^{k}(-) = -2K^{\frac{1}{2}}\epsilon_{ij}{}^{k}. \tag{5.8b}$$

The invariance of $\Omega^{\mu}_{\alpha\beta}$ under (5.1) is a consequence of $\Omega_{\mu\alpha\beta} \sim g^{\frac{1}{2}}\epsilon_{\mu\alpha\beta}$.

Since $\Gamma^{\mu}_{\alpha\beta}$ is derived from the metric, it is apparent that the connection is invariant under (5.1) and thus they constitute the generators of the group of motions of S.

If we introduce the operators

$$\tilde{X}_i(+) = \frac{1}{2iK^{\frac{1}{2}}} X_i(+), \qquad i \neq 1, \tag{5.9a}$$

$$\tilde{X}_1(+) = -\frac{1}{2iK^{\frac{1}{2}}} X_1(+), \tag{5.9b}$$

$$\tilde{X}_i(-) = \frac{1}{2iK^{\frac{1}{2}}} X_i(-), \tag{5.9c}$$

then the commutation relations take the usual form for the four-dimensional orthogonal group.

The relationship between the group of motions of S and 0_4 may be seen in another way. As regards the metric alone, the space S is that of the surface of a four-dimensional sphere since $g_{\alpha\beta}$ describes an Einstein space. Transformations of this sphere that leave the metric of its surface invariant are the rotations of the sphere about its center. These transformations belong to 0_4.

6. REPRESENTATION FUNCTIONS

We now wish to find representation functions of the group of motions on the space S. The representation functions of 0_4 on the four-dimensional Euclidian space are functions of three independent coordinates, the fourth coordinate being restricted by the condition that the radius of the sphere remain invariant. These functions are the hyperspherical harmonics and they constitute representation functions of the group of motions of S.

In general, 0_4 representations are labeled by the eigenvalues of two Casimir operators associated with the two invariant 0_3 subgroups, namely $j(j+1)$ and $j'(j'+1)$. From functions on a four-dimensional Euclidian space, only certain representations of 0_4 may be found, namely, those for which the Casimir operator eigenvalues are identical or for which $j = j'$.

In terms of the $X_i(\pm)$, the two Casimir operators are

$$\begin{aligned} \bar{g}^{ij}X_i(+)X_j(+) &\equiv X^2(+), \\ \bar{g}^{ij}X_i(-)X_j(-) &\equiv X^2(-), \end{aligned} \tag{6.1}$$

and[4] these operators are seen to be identical when expressed in terms of the λ's. Also X^2 is the Laplacian in S

$$X^2(+) = X^2(-) = \Delta = \bar{g}^{\frac{1}{2}}\,\partial_\nu(g^{\frac{1}{2}}g^{\mu\nu}\,\partial_\mu). \tag{6.2}$$

The form of the representation functions depends upon the choice of the set of eigenvalues used as labels. We are guided by the desire to make a connection with the well-known representation functions of three-dimensional Euclidian space. Consequently, the following linear and bilinear combinations of the $X_i(\pm)$ are of interest.

$$P_i = (1/i)X_i(+), \tag{6.3a}$$

$$L_i = (1/2iK^{\frac{1}{2}})[X_i(-) - X_i(+)], \tag{6.3b}$$

$$L^2 = \bar{g}^{ij}L_iL_j, \tag{6.3c}$$

$$P^2 = \bar{g}^{ij}P_iP_j = -X^2. \tag{6.3d}$$

These operators have the following commutation relations:

$$\begin{aligned} &[P_i, L_j] = i\epsilon_{ijk}P_k, && [P_i, P_j] = 2K^{\frac{1}{2}}i\epsilon_{ijk}P_k, \\ &[L_i, L_j] = i\epsilon_{ijk}L_k, && [P^2, L_i] = 0, \\ &[P^2, P_i] = 0, && [L^2, L_i] = 0, \\ &[L^2, P_i] = i\epsilon_{ijk}\{P_j, L_k\}, && [L^2, P^2] = 0. \end{aligned} \tag{6.4}$$

The operators have the property that in the limit of $K \to 0$, i.e., in the Euclidian limit, their commutation relations become those for P_i, L_i, P^2, L^2, where P_i and L_i are the usual momentum and angular momentum operators.

We are concerned with the representation functions for which the following sets of operators are diagonal

$$P^2, L^2, L_3 \tag{6.5a}$$

and

$$P^2, P_3, L_3. \tag{6.5b}$$

The functions associated with the first set correspond in Euclidian space to $j_l(kr)Y_{lm}(\theta, \phi)$. The eigenvalues of P^2, L^2, L_3 are respectively k^2, $l(l+1)$, and m.

The functions associated with the second set correspond in Euclidian space to $J_m[(k^2 - k_3^2)^{\frac{1}{2}}\rho]e^{ik_3x^3}e^{im\phi}$ with eigenvalues k^2, k_3, and m for the three operators.

7. RIEMANNIAN COORDINATE SYSTEM

We begin the study of the various differential operators of (6.5) in the Riemannian coordinate system. The vector fields $\lambda^i_\mu(\pm)$ may be expressed in this system in the following way[1]:

$$\begin{aligned} \lambda^i_\mu(\pm) &= \delta^i_\mu + \tfrac{1}{2}C_{\mu\alpha_1}{}^i(\pm)x^{\alpha_1} + \cdots \\ &\quad + [1/(r+1)!]C_{\mu\alpha_1}{}^{\beta_1}C_{\beta_1\alpha_2}{}^{\beta_2}\cdots C_{\beta_{r-1}}{}^{i}{}_{\alpha_r}x^{\alpha_1}\cdots x^{\alpha_r} \\ &= \delta^i_\mu\frac{\sin\omega}{\omega} + \omega^\mu\omega^i\frac{\omega - \sin\omega}{\omega^3} + \omega^\alpha\epsilon_{i\mu\alpha}\frac{1-\cos\omega}{\omega}, \end{aligned} \tag{7.1}$$

[4] The Killing form is identical to $\bar{g}_{ij}$.

where dimensionless coordinates ω^μ have been introduced

$$\omega^\mu = \pm 2K^{\frac{1}{2}}x^\mu \tag{7.2a}$$

and

$$\omega^2 = \sum_{\mu=1}^{3} (\omega^\mu)^2. \tag{7.2b}$$

It is seen that in the limit $K \to 0$, the λ_μ^i go to δ_μ^i. The parallel vector fields of Euclidian space are the Cartesian coordinate axes.

The other quantities of interest are

$$g_{\mu\nu} = \bar{g}_{ij}\lambda_\mu^i\lambda_\nu^j = \delta_\nu^\mu \frac{2(1 - \cos\omega)}{\omega^2} + \frac{\omega^\mu\omega^\nu}{\omega^4}(\omega^2 - 2 + 2\cos\omega), \tag{7.3}$$

$$g^{\mu\nu} = \delta_\nu^\mu \frac{\omega^2}{2(1 - \cos\omega)} + \omega^\mu\omega^\nu \frac{(2 - 2\cos\omega - \omega^2)}{2\omega^2(1 - \cos\omega)}, \tag{7.4}$$

$$\lambda_i^\mu(\pm) = \delta_i^\mu \frac{\omega\sin\omega}{2(1 - \cos\omega)} + \frac{\omega^\mu\omega^i(2 - 2\cos\omega - \omega\sin\omega)}{2\omega^2(1 - \cos\omega)} + \frac{\omega^\alpha}{2}\epsilon_{\mu\alpha i}, \tag{7.5}$$

$$P_i = \frac{1}{i}\left[\frac{\omega\sin\omega}{2(1 - \cos\omega)}\frac{\partial}{\partial x^i} + \frac{\omega^\mu\omega^i(2 - 2\cos\omega - \omega\sin\omega)}{2\omega^2(1 - \cos\omega)}\frac{\partial}{\partial x^\mu} + K^{\frac{1}{2}}x^\alpha\epsilon_{\mu\alpha i}\frac{\partial}{\partial x^\mu}\right], \tag{7.6}$$

$$L_i = \frac{1}{i}x^\alpha\epsilon_{\mu\alpha i}(\partial/\partial x^\mu) = (1/i)(x^j\,\partial_k - x^k\,\partial_j). \tag{7.7}$$

It is easily seen that as $K \to 0$, $P_i \to (1/i)(\partial/\partial x^i)$. The L_i already have the form of the angular momentum operator in Cartesian coordinates.

8. SPHERICAL WAVES

To obtain the generalization of spherical waves in S, we transform from the ω^μ system to "polar" coordinates

$$\omega = \left[\sum_{\mu=1}^{3}(\omega^\mu)^2\right]^{\frac{1}{2}},$$
$$\tan\theta = [(\omega^1)^2 + (\omega^2)^2]^{\frac{1}{2}}/(\omega^3), \tag{8.1}$$
$$\tan\phi = (\omega^2)/(\omega^1).$$

The coordinate ω is dimensionless and equals $2K^{\frac{1}{2}}r$, where r^2 is the usual sum $\sum_{\mu=1}^{3}(x^\mu)^2$. The ranges of the coordinates are

$$0 \le \omega \le 2\pi,$$
$$0 \le \theta \le \pi, \tag{8.2}$$
$$0 \le \phi \le 2\pi.$$

The Laplacian in this coordinate system takes the form,

$$\Delta = 4K\left\{\frac{\partial^2}{\partial\omega^2} + \cot\frac{\omega}{2}\frac{\partial}{\partial\omega} + \frac{1}{4\sin^2\frac{1}{2}\omega} \times \left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right\}. \tag{8.3}$$

The equation

$$P^2\psi = -X^2\psi = -\Delta\psi = Kj(j + 1)\psi \tag{8.4}$$

is solved by separation of variables to give

$$\psi_s = j_l(j, \omega)Y_{lm}(\theta, \phi), \tag{8.5}$$

where the $Y_{lm}(\theta, \phi)$ are the usual spherical harmonics and the $j_l(j, \omega)$ satisfy

$$\left\{\frac{d^2}{d\omega^2} + \cot\frac{\omega}{2}\frac{d}{d\omega} + \left[j(j + 1) - \frac{l(l + 1)}{4\sin^2\frac{1}{2}\omega}\right]\right\}j_l(j, \omega) = 0 \tag{8.6}$$

with solutions[5]

$$j_l(j, \omega) = \left[\frac{(n^2 - l^2 - 1)!}{4\pi(n^2)!}\right]^{\frac{1}{2}} \times \sin^l\frac{\omega}{2}\,d^{l+1}\frac{\cos\frac{1}{2}n\omega}{d(\cos\frac{1}{2}\omega)^{l+1}}, \tag{8.7}$$

where $n = 2j + 1$. The metric is

$$g_{\mu\nu} = \frac{1}{4K}\begin{bmatrix} 1 & & \\ & 4\sin^2(\frac{1}{2}\omega) & \\ & & 4\sin^2(\frac{1}{2}\omega)\sin^2\theta \end{bmatrix}. \tag{8.8}$$

The invariant volume element is

$$d\tau = g^{\frac{1}{2}}\,d\omega\,d\theta\,d\phi = \tfrac{1}{2}R^3\sin^2(\tfrac{1}{2}\omega)\sin\theta\,d\omega\,d\theta\,d\phi \tag{8.9}$$

and the normalization of the ψ_s over the invariant volume is taken to be unity. The operators L^2 and L_3 have the forms

$$L^2 = -\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right), \tag{8.10a}$$

$$L_3 = (1/i)(\partial/\partial\phi), \tag{8.10b}$$

and with P^2 have the eigenvalues

$$P^2 - 4Kj(j + 1),$$
$$L^2 - l(l + 1), \tag{8.11}$$
$$L^3 - m,$$

[5] These solutions are related to solutions of the hydrogen atom in momentum space; see V. Fock [Z. Physik **98**, 145 (1935)]. Schrödinger discusses these solutions in his series of articles on eigenvalue problems in a hypersphere [E. Schrödinger, Commen. Pont. Acad. Sci. **2**, 321 (1938); Proc. Roy. Irish Acad. **XLVI**, Sec. A, 9, 25 (1940)].

where j takes on nonnegative integer and half-integer values and l and m range from 0 to $2j$ and $-l$ to l, respectively, in integer steps.

The behavior of ψ_s for small K is best seen via the differential equation that the $\tilde{j}_l(j, \omega)$ functions satisfy, the Y_{lm} being unaffected in the limit $K \to 0$.

We expand (8.6) for small values of ω, keeping only lowest-order terms in ω but allowing for large j. We obtain

$$\left\{\omega^2 \frac{d^2}{d\omega^2} + 2\omega \frac{d}{d\omega} + [\omega^2 j^2 - l(l+1)]\right\}\tilde{j}_l(j, \omega) = 0 \tag{8.12}$$

with solutions $j_l(j\omega)$ or $j_l(kr)$, where $k = 2K^{\frac{1}{2}}j$.

Thus the usual momentum $k^2 = 4Kj^2$ is seen to correspond to the eigenvalue of P^2 in the limit $K \to 0$, $K^{\frac{1}{2}}j$ remaining finite.

$$P^2\psi_s = 4Kj(j+1)\psi_s \underset{j\to\infty}{\overset{K\to 0}{\to}} 4Kj^2\psi_s = k^2\psi_s. \tag{8.13}$$

The interpretation of ψ_s as a representation function of 0_4 is made by identifying ω, θ, and ϕ with the angular coordinates of a sphere in a four-dimensional Euclidian space. If y^μ are the coordinates of a unit sphere, then

$$y^1 = \sin\tfrac{1}{2}\omega \sin\theta \cos\phi, \qquad y^2 = \sin\tfrac{1}{2}\omega \sin\theta \sin\phi,$$
$$y^3 = \sin\tfrac{1}{2}\omega \cos\theta, \qquad y^4 = \cos\tfrac{1}{2}\omega, \tag{8.14}$$

where

$$\sum_{\mu=1}^{4} (y^\mu)^2 = 1. \tag{8.15}$$

9. CYLINDRICAL WAVES

The usual method of finding the cylindrical waves of Euclidian space involves a transformation to cylindrical coordinates and a separation of the Helmholtz equation in that system. The transformation from spherical coordinates is

$$x^3 = r\cos\theta, \qquad \rho = r\sin\theta, \qquad \phi = \phi. \tag{9.1}$$

The generalization of this transformation is seen as follows. On a unit three-dimensional sphere draw a meridian M through an arbitrary origin or pole. A point A in one hemisphere may be labeled by its longitude θ with respect to M and polar distance $\frac{1}{2}\omega$ or, by the shortest distance $\frac{1}{2}\beta$ from A to M, which is via the great circle C through A and perpendicular to M, and the polar distance $\frac{1}{2}\omega_3$ of the intersection M and C. To make the labeling unique, points of $\theta < \frac{1}{2}\pi$ have $\omega_3 > 0$ and points of $\theta > \frac{1}{2}\pi$ have $\omega_3 < 0$. β is seen to range from 0 to π and ω_3 from -2π to 2π. The relationship between the coordinate systems is (see Fig. 1)

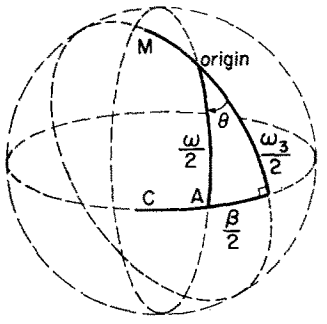

FIG. 1. Relationship between "polar" and "cylindrical" coordinates.

$$\sin\tfrac{1}{2}\beta = \sin\tfrac{1}{2}\omega \sin\theta,$$
$$\tan\tfrac{1}{2}\omega_3 = \tan\tfrac{1}{2}\omega\cos\theta, \tag{9.2}$$
$$\phi = \phi.$$

Equations (9.2) reduce to (9.1) in the limit $K \to 0$. Here $\beta = 2K^{\frac{1}{2}}\rho$ and $\omega_3 = \omega^3 = 2K^{\frac{1}{2}}x^3$.

The equation

$$[\Delta + 4Kj(j+1)]\psi = 0 \tag{9.3}$$

now takes the form

$$\left[\frac{\partial^2}{\partial\beta^2} + \cot\beta\frac{\partial}{\partial\beta} + \frac{1}{\cos^2(\frac{1}{2}\beta)}\frac{\partial^2}{\partial\omega_3^2} + \frac{1}{4\sin^2(\frac{1}{2}\beta)}\frac{\partial^2}{\partial\phi^2} + j(j+1)\right]\psi_c = 0 \tag{9.4}$$

with solutions

$$\psi_c = \tilde{J}_m(j, s; \beta)e^{is\omega_3}e^{im\phi}, \tag{9.5}$$

where $\tilde{J}_m(j, s; \beta)$ satisfies

$$\left\{\frac{d^2}{d\beta^2} + \cot\beta\frac{d}{d\beta} - \frac{1}{\sin^2\beta}\left[2s^2 + \frac{m^2}{2} - \cos\beta\left(2s^2 - \frac{m^2}{2}\right)\right] + j(j+1)\right\}\tilde{J} = 0. \tag{9.6}$$

With the substitution

$$s = \tfrac{1}{2}(\mu + \nu), \tag{9.7a}$$
$$m = -\mu + \nu, \tag{9.7b}$$

Eq. (9.6) takes the form

$$[(d^2/d\beta^2) + \cot\beta - (1/\sin^2\beta) \times (\mu^2 + \nu^2 - 2\mu\nu\cos\beta) + j(j+1)]\tilde{J} = 0 \tag{9.8}$$

with solutions

$$J_m(j, s; \beta) \sim d^j_{\mu\nu}(\beta), \tag{9.9}$$

where the $d^j_{\mu\nu}(\beta)$ are the familiar functions of the finite representation theory of 0_3.

The complete solutions may be put into the form of the $D^j_{\mu\nu}(\alpha, \beta, \gamma)$ functions as follows:

$$\psi_c = \tilde{J}_m(j, s; \beta)e^{is\omega_3}e^{im\phi} = (-1)^{\mu+\nu}Nd^j_{\mu\nu}(\beta)e^{i\mu\alpha}e^{i\nu\gamma} = (-1)^{\mu+\nu}ND^j_{\mu\nu}(\alpha, \beta, \gamma), \tag{9.10}$$

where

$$\gamma = \tfrac{1}{2}\omega_3 + \phi + \pi, \tag{9.11a}$$

$$\alpha = \tfrac{1}{2}\omega_3 - \phi + 3\pi, \tag{9.11b}$$

and

$$\begin{aligned} 0 \le \alpha \le 4\pi, \\ 0 \le \gamma \le 4\pi. \end{aligned} \tag{9.12}$$

N is a normalization factor which is now computed. The metric takes the form

$$g_{\mu\nu} = \frac{1}{4K}\begin{bmatrix} 1 & & \\ & \cos^2(\tfrac{1}{2}\beta) & \\ & & 4\sin^2(\tfrac{1}{2}\beta) \end{bmatrix} \tag{9.13}$$

with the invariant volume element given by (here $R^2 = K^{-1}$)

$$d\tau = g^{\frac{1}{2}}\, d\beta\, d\omega_3\, d\phi = \tfrac{1}{8}R^3 \sin\beta\, d\beta\, d\omega_3\, d\phi. \tag{9.14}$$

We have

$$\begin{aligned} &\delta_{jj'}\,\delta_{ss'}\,\delta_{mm'} \\ &= \frac{R^3}{8}|N|^2 \int_0^{\pi}\int_{-2\pi}^{2\pi}\int_0^{2\pi} \sin\beta (d^{j'}_{\mu'\nu'} e^{is'\omega_3} e^{im'\phi})^* \\ &\quad \times (d^{j}_{\mu\nu} e^{is\omega_3} e^{im\phi})\, d\beta\, d\omega_3\, d\phi \\ &= R^3 |N|^2 \pi^2\, \delta_{ss'}\,\delta_{mm'} \int_0^{\pi} \sin\beta d^{*j'}_{\mu\nu}\, d^{j}_{\mu\nu}\, d\beta \\ &= \frac{2\pi^2 R^3 |N|^2}{2j+1}\,\delta_{jj'}\,\delta_{ss'}\,\delta_{mm'} \end{aligned} \tag{9.15}$$

or

$$N = \left(\frac{2j+1}{2\pi^2 R^3}\right)^{\frac{1}{2}} = \left(\frac{2j+1}{V}\right)^{\frac{1}{2}}, \tag{9.16}$$

where V is the total volume of S. The last integration is based on the orthogonality of the $d^j_{\mu\nu}$.

The operators P^2, P_3, L_3 have eigenvalues $4Kj(j+1)$, $2K^{\frac{1}{2}}\mu = 2K^{\frac{1}{2}}(s - \frac{1}{2}m)$, and $-\mu + \nu = m$, where μ and ν have the ranges $-j \le \begin{matrix}\mu\\\nu\end{matrix} \le j$ in integer steps.

The equation for $\tilde{J}$ may be expanded for small K, or β, keeping only lowest-order terms but allowing for large j and s.

We have from (9.6),

$$\left(\frac{d^2}{d\beta^2} + \frac{1}{\beta}\frac{d}{d\beta} + j^2 - s^2 - \frac{m^2}{\beta^2}\right)\tilde{J} = 0$$

or Bessel's equation with solutions $J_m[(j^2 - s^2)^{\frac{1}{2}}\beta]$. The argument is $(k^2 - k_3^2)^{\frac{1}{2}}\rho$, where $k^2 = 4j^2K$ and $k_3 = 2K^{\frac{1}{2}}s$.

10. PLANE WAVES

We are now in a position to see the generalization of the plane wave of flat space. The wave $J_m[(k^2 - k_3^2)^{\frac{1}{2}}\rho]e^{ik_3x^3}e^{im\phi}$ reduces to a plane wave in the three-direction when k_3 assumes its maximum value and when $m = 0$. The same two conditions when applied to the generalized cylindrical wave define a function which we call a generalized plane wave. Thus the plane wave is

$$\begin{aligned} \psi_P &= [(2j+1)/V]^{\frac{1}{2}}\, d^j_{ii}\,(\beta) e^{ij\omega_3} \\ &= [(2j+1)/V]^{\frac{1}{2}} \cos^{2j}(\tfrac{1}{2}\beta) e^{ij\omega_3}. \end{aligned} \tag{10.1}$$

When expressed in terms of the dimensional coordinates and expanded for large R, we have

$$\begin{aligned} \psi_P &= \left(\frac{2j+1}{V}\right)^{\frac{1}{2}}\left(1 - \sin^2\frac{\rho}{R}\right)^j e^{ik_3x^3} \\ &\to \left(\frac{k_3}{RV}\right)^{\frac{1}{2}} e^{ik_3x^3}\left(1 - \frac{k_3\rho^2}{2R} + \cdots\right). \end{aligned} \tag{10.2}$$

11. EINSTEIN SPACE

As shown earlier, the space defined by $g_{\alpha\beta}$ and $\Gamma^{\mu}_{\alpha\beta}$ is the Einstein space. Its group of motions is the same as that of $S^{(2)}$. Thus, the above functions are also representation functions of the group of motions of the Einstein space on the space itself.

In the case of S, K is a measure of the torsion, there being no curvature to the space. In the case of the Einstein space, K is a measure of the curvature of the space, the torsion being zero.

12. SUMMARY

The space described here is in several ways a convenient one to describe physical space. The observed Hubble effect may be given an interpretation in terms of either an expanding Einstein space or an expanding Clifford space. Also, coordinate reflections do not take the space into itself and consequently, linear equations involving the operators $X_i(\pm)$ are not invariant under parity operations.[6] Such a situation is interesting from the point of view of the description of processes in which parity is not conserved or is only partially conserved, such as in weak interactions.

The functions discussed in this paper are basis functions for a description of quantization in Clifford space. The scalar field theory generalizes to Clifford space with no difficulty.[7] Spinor quantization problems are now being investigated by the author.[8]

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Role of the Integral-Operator Method in the Theory of Potential Scattering*

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A recently developed method in the theory of potential scattering is investigated. The authors supply analytic computations for determining the location and the type of singularities, which occur in several scattering amplitudes that are constructed from physically relevant potentials.

IN a paper by Gilbert and Shieh,[1] a new method for investigating the analytic properties of the scattering amplitude $A(k, \cos\theta)$ was given. Their results depended upon the fact that there exist an integral operator $\Omega[B]$ and its inverse $\Omega^{-1}[A]$ which map the following two series,

$$B(k, z) = \sum_{l=0}^{\infty} a_l(k) z^l, \tag{1}$$

$$A(k, z) = \sum_{l=0}^{\infty} a_l(k) P_l(z), \tag{2}$$

onto one another, i.e.,

$$A(k, z) = \Omega[B] \equiv \frac{1}{2\pi i} \int_{|\zeta|=1} B\left[k, z + \frac{1}{2}\left(\zeta + \frac{1}{\zeta}\right)(z^2 - 1)^{\frac{1}{2}}\right] \frac{d\zeta}{\zeta}, \tag{3}$$

and

$$B(k, z) = \Omega^{-1}[A] \equiv \tfrac{1}{2}(1 - z^2) \int_{-1}^{+1} \frac{A(k, \xi)\, d\xi}{(1 - 2\xi z + z^2)^{\frac{3}{2}}}. \tag{4}$$

By using both operators, they were able to list theorems concerning the location, the number, and the type of singularities the scattering amplitude could have by comparing it with its associate function $B(k, z)$. The reader is referred to the paper mentioned above, to the original paper by Nehari[2] concerning the location of singularities of Legendre series, and to the book by Bergman,[3] who pioneered the research in this area.

The advantage of the method given by Gilbert and Shieh over that used by Regge[4] is that information concerning the analytic properties of the scattering amplitude can be obtained directly from the partial wave amplitudes without the continuation of the angular momentum from physical values to complex ones. In this paper, we illustrate the method of Gilbert and Shieh by considering some potentials of physical interest.

Newton[5] gives the following asymptotic expression for the partial wave amplitudes as $l \to \infty$,

$$a_l(k) \approx -i\pi \int_0^{\infty} V(r)[J_l(kr)]^2 r\, dr, \tag{5}$$

which is valid when $V(r) \approx O(e^{-\mu r})$ as $r \to \infty$, where $V(r)$ is the potential, and $J_l(z)$ is a Bessel function of the first kind and of the lth order. From the literature on Bessel functions,[6] it is possible to list the asymptotic forms of several partial wave amplitudes; this is done in Table I. We remark that the inverse square potential (4) is actually contained in Eq. (2), although it is listed separately. The superposition of Yukawa potentials (5) and the Coulomb potential (7) were not obtained by direct integration and we owe these results to Newton.[7] We have added them because they are of general interest. The cases (2) and (4) are merely the Born approximations for the partial wave amplitudes; hence our corresponding computations of the singularities are only estimates.

We are able to locate the singularities of the function $B(k, z)$ in the z plane by using the Hadamard formula for the radius of convergence (in the z plane),

$$\frac{1}{\rho(k)} = \limsup_{l\to\infty} |a_l(k)|^{1/l}, \tag{6}$$

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[1] R. P. Gilbert and S. Y. Shieh, Technical Note BN-401, Institute for Fluid Dynamics and Applied Mathematics, University of Maryland, 1965.

[2] Z. Nehari, J. Ratl. Mech. Anal., 5, 987 (1956).

[3] S. Bergman, *Integral Operators in the Theory of Linear Partial Differential Equations* (Springer-Verlag, Berlin, 1960).

[4] T. Regge, Nuovo Cimento **14**, 951 (1959).

[5] R. Newton, *The Complex j-plane* (W. A. Benjamin, Inc., New York, 1964), p. 42.

[6] G. N. Watson, *A Treatice on the Theory of Bessel Functions* (Cambridge University Press, New York, 1944), See in particular pp. 395, 399, 403, 411.

[7] See Ref. 5 pp. 44 and 86.

TABLE I. Asymptotic forms of several partial wave amplitudes.

	Scattering potential	Partial wave amplitude as $l \to \infty$
1.	$e^{-a^2r^2}$	$(-i\pi/2a^2)e^{-k^2/a^2}I_l(k^2/2a^2)$
2.	$r^{-\alpha-1}$, Re $\alpha > 0$	$-i\pi\left(\frac{k}{2}\right)^{\alpha-1} \frac{\Gamma(\alpha)\Gamma(l+\frac{1}{2}[1-\alpha])}{2\Gamma(\frac{1}{2}[\alpha+1])^2\Gamma(l+\frac{1}{2}[\alpha+1])}$
3.	$r^{\alpha-2}e^{-a^2r^2}$	$\frac{-i\pi k^{2l}}{2^{2l}a^{2l+\alpha}} \frac{\Gamma(l+\frac{1}{2}\alpha)}{\Gamma(l+1)^2}$ $\times {}_2F_2(l+\frac{1}{2}, l+\alpha/2; l+1, 2l+1; -k^2/a^2)$
4.	r^{-2}	$-i/2l$
5.	$e^{-\mu_0 r}/r$	$(-i/k)Q_l(1+\mu_0/2k^2)$
6.	$\int_{\mu_0}^{\infty} \rho(\mu) \frac{e^{-\mu r}}{r} d\mu$, $\mu_0 > 0$	$l^{-\frac{1}{2}}[(\mu_0/2k)+(1+\mu_0^2/4k^2)^{\frac{1}{2}}]^{-2l}$
7.	r^{-1}	$\frac{\Gamma(l+1+i\gamma)}{\Gamma(l+1-i\gamma)}$, $\gamma = +C/k$, where C is the strength of the Coulomb potential.

and the Fabry formula,[8]

$$\lim_{l\to\infty} \frac{a_l(k)}{a_{l+1}(k)} = \rho(k)e^{i\theta(k)}, \tag{7}$$

when the indicated limit exists. Providing $z \neq \pm 1$, the singularities of $A(k, z)$ are then related to those of $B(k, z)$ by the formula[9]

$$z = \tfrac{1}{2}[\xi(k) + 1/\xi(k)], \tag{8}$$

where $\xi(k) = \rho(k)e^{i\theta(k)}$. Using formulas (6)–(8), we are able to compute the singularities of $B(k, z)$ and $A(k, z)$. We list these singularities in Table II.

In the case of (1), we use the asymptotic estimate,[10]

$$I_l(z) \approx 2(\pi)^{-\frac{1}{2}}\{\sqrt{2}\,(l^2+z^2)^{-\frac{1}{4}} \times \exp[(l^2+z^2)^{\frac{1}{2}} - l\sinh^{-1}(l/z)]\} \times \{1 + O(1/l)\}, \quad z > 0,$$

hence

$$\lim_{l\to\infty} \frac{1}{l} \log I_l(z) = -\lim_{l\to\infty} [\sinh^{-1}(l/z)] = -\infty.$$

In this case, we have the scattering amplitude

$$A(k, z) = \frac{1}{2a^2} e^{-k^2/2a^2} \sum_{l=1}^{\infty} I_l(k^2/2a^2)P_l(z) \tag{9}$$

converges everywhere in the z plane for k in the physical range.

The case (2) is estimated as follows. Since, for arbitrary complex α, β,[11]

$$\frac{\Gamma(l+\alpha)}{\Gamma(l+\beta)} \approx l^{\alpha-\beta}\left[1 + \frac{1}{2l}(\alpha^2 - \beta^2) + O\left(\frac{1}{l^2}\right)\right],$$

we have

$$a_l(k) \approx \left(\frac{k}{2}\right)^{\alpha} \frac{\Gamma(\alpha)}{2\Gamma\left(\frac{\alpha+1}{2}\right)^2} l^{-\alpha}\left[1 + O\left(\frac{1}{l^2}\right)\right],$$

and consequently

$$\frac{a_l(k)}{a_{l+1}(k)} \approx \frac{l^{-\alpha}}{(l+1)^{-\alpha}} \to 1 \quad \text{as} \quad l \to \infty.$$

The case of (4) is contained in the case of (2).

Case (7) can be handled similarly by noting that as $l \to \infty$,

$$a_l(k) \approx \frac{\Gamma(l+1+i\gamma)}{\Gamma(l+1-i\gamma)} \approx (l+1)^{2i\gamma}\left[1 - \frac{i\gamma}{l+1} + O\left(\frac{1}{l^2}\right)\right].$$

Hence, $a_{l+1}(k)/a_l(k) \approx 1 + O(1/l)$, and we realize that $z = 1$ is a singular point.

In order to treat the case of (3), we must ob-

[8] P. Dienes, *The Taylor Series* (Oxford University Press, London, 1931), p. 377.

[9] See Refs. 1 and 2. In Ref. 1, it is shown that $A(k, z)$ may be singular at $z = +1$ without corresponding to a singularity of $B(k, z)$.

[10] *Bateman Manuscript Project, Higher Transcendental Functions*, A. Erdelyi, Ed. (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, p. 86.

[11] See Vol. I of Ref. 10, p. 47.

TABLE II. Singularities of $B(k, z)$ and $A(k, z)$.

	Scattering potential	Singularity in z plane of $B(k, z)$	Singularity in z plane of $A(k, z)$
1.	$e^{-a^2r^2}$	∞	∞
2.	$r^{-\alpha-1}$, $\operatorname{Re}\alpha > 0$	1	1
3.	$r^{\alpha-2}e^{-a^2r^2}$	∞	∞
4.	r^{-2}	1	1
5.	$e^{-\mu_0 r}/r$	$(\mu_0/2k) + (1 + \mu_0^2/4k^2)^{\frac{1}{2}}$, $\lvert k\rvert < \mu_0$	$(1 + \mu_0^2/4k^2)^{\frac{1}{2}}$
6.	$\int_{\mu_0}^{\infty} \rho(\mu)\frac{e^{-\mu r}}{r}\,d\mu$, $\mu_0 > 0$	$(\mu_0/2k) + (1 + \mu_0^2/4k^2)^{\frac{1}{2}}$, $\lvert k\rvert < \mu_0$	$(1 + \mu_0^2/4k^2)^{\frac{1}{2}}$
7.	r^{-1}	1	1

tain an asymptotic expression for ${}_2F_2(l + 1/2, l + \alpha/2; l + 1, 2l + 1; -k^2/a^2)$, which is a generalized hypergeometric function.[12] We consider the generalized hypergeometric function[13]

$$ {}_2F_2(l + a_1, l + a_2; l + c_1, 2l + c_2; z) = \sum_{n=0}^{\infty} \frac{(l + a_1)_n(l + a_2)_n}{(l + c_1)_n(2l + c_2)_n}\frac{z^n}{n!}, $$

where $(\alpha)_n \equiv \alpha(\alpha + 1)\cdots(\alpha + n - 1)$, $n \geq 1$, and $(\alpha)_0 \equiv 1$. We note that the general term of the series can be rewritten as

$$ \frac{(l + a_1)_n(l + a_2)_n}{(l + c_1)_n(l + c_2)_n}\frac{z^n}{n!} = \left(\frac{z}{2}\right)^n \frac{1}{n}\left\{\left(1 + \frac{\alpha}{l + c_1}\right)\left[\frac{1}{\sqrt{2}} + \frac{\alpha}{(l + c_1 + 1)\sqrt{2}}\right]\cdots \right. $$
$$ \times \left.\left[\frac{1}{(n-1)^{\frac{1}{2}}} + \frac{\alpha}{(l + c_1 + n - 1)(n-1)^{\frac{1}{2}}}\right]\right\} $$
$$ \times \left\{\left(1 + \frac{\beta}{l + \frac{1}{2}c_2}\right)\left[\frac{1}{\sqrt{2}} + \frac{\beta + \frac{1}{2}}{[l + \frac{1}{2}(c_2 + 1)]\sqrt{2}}\right]\cdots \right. $$
$$ \times \left.\left[\frac{1}{(n-1)^{\frac{1}{2}}} + \frac{\beta + \frac{1}{2}(n-1)}{[l + \frac{1}{2}(c_2 + n - 1)](n-1)^{\frac{1}{2}}}\right]\right\}, $$

where $\alpha \equiv a_1 - c_1$, $\beta \equiv a_2 - \frac{1}{2}c_2$. Now, let m be the smallest positive integer such that

$$ 0 < \delta \equiv \gamma\left[\frac{1}{(m-1)^{\frac{1}{2}}} + \frac{\alpha}{(m-1)^{\frac{1}{2}}(l + c_1 + m - 1)}\right] \times \left[\frac{1}{(m-1)^{\frac{1}{2}}} + \frac{\beta/(m^{\frac{1}{2}}) + \frac{1}{2}(m-1)^{\frac{1}{2}}}{l + \frac{1}{2}(c_2 + m - 1)}\right] < 1, $$

where $\lvert z/2\rvert < \gamma$. Then, if $\nu \geq m$, the remainder of the series,

$$ \left|\sum_{n\geq\nu}^{\infty} \frac{(l + a_1)_n(l + a_2)_n}{(l + c_1)_n(2l + c_2)_n}\frac{z^n}{n!}\right| \leq \frac{1}{\nu}\left\{\left[1 + \frac{\alpha}{l + c_1}\right]\cdots\left[\frac{1}{(m-1)^{\frac{1}{2}}} + \frac{\alpha}{(m-1)^{\frac{1}{2}}(l + c + m - 1)}\right]\right\} $$
$$ \times \left\{\left[1 + \frac{\beta}{(l + \frac{1}{2}c_2)}\right]\cdots\left[\frac{1}{(m-1)^{\frac{1}{2}}} + \frac{\beta(m-1)^{-\frac{1}{2}} + \frac{1}{2}(m-1)^{\frac{1}{2}}}{l + \frac{1}{2}(c_2 + m - 1)}\right]\right\}\gamma^m \sum_{n=\nu}^{\infty}\delta^{n-m}, $$

which tends to 0 as $\nu \to \infty$ for l sufficiently large. Hence, we conclude that

$$ \lim_{l\to\infty} {}_2F_2(l + a_1, l + a_2; l + c_1, 2l + c_2; -k^2/a^2) = e^{-k^2/2a^2} \tag{10} $$

for k contained in a compact set. From this, we have

$$ \overline{\lim_{l\to\infty}}\,|a_l|^{1/l} \equiv \overline{\lim_{l\to\infty}}\left|\frac{\pi k^{2l}}{2^{2l}a^{2l+\alpha}}\frac{\Gamma(l + \alpha/2)}{\Gamma(l + 1)^2}\,{}_2F_2\left(l + \tfrac{1}{2}, l + \alpha/2; l + 1, 2l + 1; \frac{-k^2}{a^2}\right)\right|^{1/l} \to 0, \tag{11} $$

since, as $l \to \infty$,

$$ \frac{1}{l}\log|a_l| \approx 2\log\frac{k}{2a} + \frac{1}{l}\left\{\left(\frac{\alpha}{2} - 1\right)\right. $$
$$ \times \left.\log l + \log[1 + O(\tfrac{1}{2})] - \log\Gamma(l + 1)\right\} $$

and $1/l \log \Gamma(l + 1) \approx \log l - 1 + O(1/l)$.

We conclude that the scattering amplitude

$$ A(k, z) = \frac{i\pi}{a^\alpha}\sum_{l=0}^{\infty}\left(\frac{k}{2a}\right)^l \frac{\Gamma(l + \alpha/2)}{\Gamma(l + 1)^2} \times {}_2F_2\left(l + \tfrac{1}{2}, l + \frac{\alpha}{2}; l + 1, 2l + 1, \frac{-k^2}{a^2}\right)P_l(z) \tag{12} $$

is regular for all z and k in any compact set of $\mathbf{C}^2$, since the estimate (10) holds for all $k \neq \infty$.

[12] See Vol. I of Ref. 10, Chap. IV.
[13] See Vol. I of Ref. 10, p. 76.

The case of (5) is handled by making use of the asymptotic expression

$$Q_l(z) \approx \left[1 + O\left(\frac{1}{l}\right)\right] \times \left(\frac{\pi}{2}\right)^{\frac{1}{2}} \frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})} \frac{(z^2-1)^{-\frac{1}{4}}}{[z+(z^2-1)^{\frac{1}{2}}]^{l+\frac{1}{2}}},$$

which leads to

$$a_l(k) \approx \frac{-i}{k} Q_l\left(1 + \frac{\mu_0}{2k^2}\right) \approx \frac{-i}{k}\left(\frac{\pi}{2}\right)^{\frac{1}{2}} l^{-\frac{1}{4}} \times \left[\frac{\mu_0}{2k} + \left(1 + \frac{\mu_0^2}{4k^2}\right)^{\frac{1}{2}}\right]^{-2l-1}.$$

Newton obtains the asymptotic form for the case of (6) (which contains the above if a Stieltjes measure is used) in the same way. His result for (6) is

$$a_l(k) \approx \text{const } l^{-\frac{1}{4}}[(\mu_0/2k) + (1 + \mu_0^2/4k^2)^{\frac{1}{2}}]^{-2l-1}, \quad (13)$$

where μ_0 is the lower integration limit. By using the Hadamard and the Fabry theorems, we realize that the first singularity in the z plane of $B(k, z)$ is located at

$$z = (\mu_0/2k) + (1 + \mu_0^2/4k^2)^{\frac{1}{2}}.$$

Hence, by Eq. (8), $A(k, z)$ must be singular at

$$z = (1 + \mu_0^2/4k^2)^{\frac{1}{2}}. \quad (14)$$

In the paper by Gilbert and Shieh, a method was given for obtaining the type and the numbers of singularities of the functions $A(k, z)$ in the z plane. (The reader is directed to Gilbert,[14] and Gilbert and Howard[15] for further details of this method.) It was shown that, by considering the following lim sup,

$$L_\mu \equiv \limsup_{l\to\infty} |D_l^{(k)}|^{1/l}, \quad (15)$$

where

$$D_l^{(\nu)}(k) \equiv \begin{vmatrix} a_l(k), & \cdots, & a_{l+\mu}(k) \\ \vdots & & \\ a_{l+\mu}(k), & \cdots & a_{l+2\mu}(k) \end{vmatrix}, \quad (16)$$

one could obtain information concerning the number of singularities in certain ellipses of the z plane. For instance, if

$$\limsup_{l\to\infty} |a_l(k)|^{1/l} \to \frac{1}{\rho},$$

and we define the ellipse $E(\rho)$ as the set of points $z \equiv (x, y)$ such that

$$\frac{x^2}{(\rho - 1/\rho)^2} + \frac{y^2}{(\rho + 1/\rho)^2} \leq \frac{1}{4},$$

then, depending on whether the ratios $L_\nu/L_{\nu-1}$ are (1) equal to zero for all $\nu \geq N$, (2) tend to zero as $\nu \to \infty$, (3) tend to $1/\rho$ as $\nu \to \infty$, or (4) equal to $1/\rho$ for all $\nu \geq N$, for some $N \geq 0$, we have the following corresponding possibilities for the singular behavior of $A(k, z)$: (1) there are at most N polelike branch points in the entire z plane, (2) there are just a finite number of polelike branch points in every compact set of the z plane, (3) there are a finite number of polelike branch points in the ellipse $E(\rho - \epsilon)$, $0 < \epsilon < \rho$, but an infinite number in a neighborhood of $E(\rho)$, and (4) the singularity, in general, is not a polelike branch point.

To illustrate this result, we consider cases (6) and (7), where

$$a_l(k) \approx \text{const } l^{-\frac{1}{4}}\, \delta^{-2l-1},$$

for l sufficiently large and

$$\delta \equiv (\mu_0/2k) + (1 + \mu_0^2/4k^2)^{\frac{1}{2}}.$$

This leads us to consider the determinants $D_l^{(\nu)}(u)$,

$$D_l^{(\nu)}(k) \equiv \begin{vmatrix} (l)^{-\frac{1}{4}}, & (l+1)^{-\frac{1}{4}}, & \cdots, & (l+\nu)^{-\frac{1}{4}} \\ (l+1)^{-\frac{1}{4}}, & \cdots & & \\ \vdots & & & \\ (l+\nu)^{-\frac{1}{4}}, & \cdots, & & (l+2\nu)^{-\frac{1}{4}} \end{vmatrix}. \quad (17)$$

We may rewrite (17) as

$$D_l^{(\nu)}(k) = l^{-\frac{1}{4}(\nu+1)} \begin{vmatrix} 1, & (1+1/l)^{-\frac{1}{4}}, & \cdots, & (1+\nu/l)^{-\frac{1}{4}} \\ (1+1/l)^{-\frac{1}{4}}, & \cdots, & & \\ \vdots & & & \\ (1+\nu/l)^{-\frac{1}{4}}, & \cdots, & & (1+2\nu/l)^{-\frac{1}{4}} \end{vmatrix}.$$

[14] R. P. Gilbert, J. Math. Phys. 5, 983 (1964).
[15] R. P. Gilbert and H. C. Howard, Proc. London Math. Soc., 15, 346 (1965).

For l sufficiently large, we have

$$D_l^{(\nu)}(k) = l^{-\frac{1}{2}(\nu+1)} \begin{vmatrix} 1, & \sum_{i=0}^{\infty} C_i^{-\frac{1}{2}} \left(\frac{1}{l}\right)^i, \cdots, & \sum_{i=0}^{\infty} C_i^{-\frac{1}{2}} \left(\frac{\nu}{l}\right)^i \\ \vdots & & \\ \sum_{i=0}^{\infty} C_i^{-\frac{1}{2}} \left(\frac{\nu}{l}\right)^i, \cdots, & & \sum_{i=0}^{\infty} C_i^{-\frac{1}{2}} \left(\frac{2\nu}{l}\right)^i \end{vmatrix}.$$

However, $D_l^{(\nu)}(k) \equiv P(a_0, a_1, \cdots, a_n)$ is a *persymmetric* determinant, and it is well known[16] that

$$P(a_0, a_1, \cdots, a_n) = P(a_0, \Delta a_1, \Delta^2 a_2, \cdots, \Delta^n a_n), \qquad \text{where} \qquad \Delta^k a_i = \Delta(\Delta^{k-1} a_i),\ \Delta^1 a_i = a_i - a_{i-1}.$$

Applying this result to $D_l^{(\nu)}(k)$ above yields

$$D_l'(k) = l^{-\frac{1}{2}(\nu+1)} \begin{vmatrix} 1, & C_1^{-\frac{1}{2}} \frac{1!}{l} + O\left(\frac{1}{l^2}\right), \cdots, & C_\nu^{-\frac{1}{2}} \frac{\nu!}{l^\nu} + O\left(\frac{1}{l^{\nu+1}}\right) \\ C_1^{-\frac{1}{2}} \frac{1!}{l} + O\left(\frac{1}{l^2}\right), \cdots, & & \\ C_\nu^{-\frac{1}{2}} \frac{\nu!}{l^\nu} + O\left(\frac{1}{l^{\nu+1}}\right), \cdots, & & C_{2\nu}^{-\frac{1}{2}} \frac{(2\nu)!}{l^{2\nu}} + O\left(\frac{1}{l^{2\nu+1}}\right) \end{vmatrix}. \tag{18}$$

Factoring $1/l$ from column 2, $1/l^2$ from column 3, ..., $1/l^\nu$ from column $\nu + 1$, and, in addition, factoring $1/l$ from row 2, $1/l^2$ from row 3, ..., etc., we obtain

$$D_l^{(\nu)}(n) = l^{-\frac{1}{2}(\nu+1)}(l^{1+2+\cdots+\nu})^{-1}(l^{1+2+\cdots+\nu})^{-1} \times \begin{vmatrix} 1, & C_1^{-\frac{1}{2}} + O(1/l), & C_2^{-\frac{1}{2}} 2! + O(1/l), \cdots, C_\nu^{-\frac{1}{2}} \nu! + O(1/l) \\ C_1^{-\frac{1}{2}} + O(1/l), \cdots & & \\ C_\nu^{-\frac{1}{2}} \nu! + O(1/l), \cdots & & C_{2\nu}^{-\frac{1}{2}} (2\nu)! + O(1/l) \end{vmatrix}.$$

From the structure of this last determinant, it is clear that we can write $D_l'(k) = l^{-(\nu+1)(\nu+1/2)}[C_0 + O(1/l)]$, where C_0 is the persymmetric determinant, with

$$C_0 = \begin{vmatrix} 1 & C_1^{-\frac{1}{2}} \cdot 1!, \cdots, & C_\nu^{-\frac{1}{2}} \cdot \nu! \\ \vdots & & \\ C_\nu^{-\frac{1}{2}} \nu!, & & C_{2\nu}^{-\frac{1}{2}} \cdot (2\nu)! \end{vmatrix}.$$

By elementary factoring methods, this can be shown to be equal to

$$C_0 = (-1)^{\frac{1}{2}\nu(\nu+1)}(1)(1\cdot 3)(1\cdot 3\cdot 5)\cdots(1\cdot 3\cdot 5\cdots[2\nu-1]) \times \begin{vmatrix} 1, -1, & 1\cdot 3, & \cdots (-1)^\nu 1\cdot 3\cdot 5\cdots(2\nu-1) \\ 1, -3, & 3\cdot 5, & \cdots (-1)^\nu 3\cdot 5\cdot 7\cdots(2\nu+1) \\ \vdots & & \\ 1, -(2\nu+1), & (2\nu+1)(2\nu+3), & \cdots (-1)^\nu (2\nu+1)\cdots(4\nu-1) \end{vmatrix}.$$

If one now operates on this last determinant with the following operations: row (n) − row $(n-1)$, row $(n-1)$ − row $(n-2)$, ..., row (2) − row (1), and then if one performs on the resulting determinant the operations row (n) − row $(n-1)$, ..., row (3) − row (2), and so on (there being one less operation each time), and since $\Delta^i(2\nu+1)(2\nu+3)\cdots(2\nu+(2j-1)) = 2^i j!$, one obtains

[16] A. C. Aitken, *Determinants and Matrices* (Interscience Publishers, Inc., New York, 1951), p. 122.

$$C_0 = (-1)^{\frac{1}{2}[\nu(\nu+1)]}1(1\cdot 3)\cdots(1\cdot 3\cdot 5\cdots[2\nu-1])$$

$$\times \begin{vmatrix} 1 & x & x & x & x & x \\ 0 & -2\cdot 1! & x & x & x & x \\ 0 & 0 & +2^2\cdot 2! & x & x & x \\ 0 & 0 & 0 & -2^3\cdot 3! & x & \\ 1 & \cdots & 0 & 0 & & \\ \cdot & & & & \cdot & x \\ \cdot & & & & 0, & (-1)^i 2^i j! \\ \cdot & & & & & \cdot \\ 0 & & \cdots & & & 0, (-1)^\nu 2^\nu \nu! \end{vmatrix}$$

$$= 2^{-\frac{1}{2}[\nu(\nu+1)]}(1)(1\cdot 3)(1\cdot 3\cdot 5)\cdots(1\cdot 3\cdot 5\cdot\cdots[2\nu-1])1!\,2!\cdots\nu!, \qquad (19)$$

hence,

$$D_l^{(\nu)}(k) = (C_0/l^{[\nu^2+\frac{1}{2}(\nu+1)]})[1 + O(1/l)], \qquad (20)$$

where C_0 is independent of l, as is shown above. Hence, we have the result that

$$\limsup_{l\to\infty} |D_l^{(\nu)}|^{1/l} = \lim_{l\to\infty} \left| \frac{C_0}{l^{[\nu^2+\frac{1}{2}(\nu+1)]}} \left[1 + O\left(\frac{1}{l}\right)\right] \right|^{1/l}$$

$$\equiv 1 \quad \text{for all} \quad \nu \geq 0.$$

It follows then that $L_\nu/L_{\nu-1} = 1$ for all $\nu \geq 1$, which rules out the possibility of $A(k, z)$ having a polelike branch point at $z = (1 + \mu_0/4k^2)^{\frac{1}{2}}$. We conclude that $B(k, z)$ has a nonpolar singularity, since $L_\nu/L_{\nu-1}$ is monotone decreasing and only Eq. (4) contains the situation described above. That this is indeed true is shown below by using known information concerning a related function.

We remark at this point that we can easily determine the behavior of $B_0(k, z)$ about its singularity at $z = \delta^2$, because of its relation to the generalized zeta function,[17]

$$F(z, s) = \sum_{l=1}^{\infty} \frac{z^l}{l^s},$$

whose singularity at $z = 1$ has logarithmic branching and whose continuation across $[1, \infty)$ is well known. If $B_0(k, z)$ is the principal branch correspond to the series representation above, and $B_1(k, z)$ is the continued function obtained by crossing over the cut $\Lambda \equiv \{z \mid z = \delta^2 + i\lambda; \lambda \geq 0\}$ from the left to the right, then one has[18] [by rotating coordinates and choosing the principal branch to be defined for arg $(z - \delta^2)$ between $\frac{1}{2}\pi$ and $5\pi/2$],

$$B_1(k, z) = B_0(k, z) + [\pi/(2 \log \delta e^{i\pi/4} - \log z)]^{\frac{1}{2}}.$$

Crossing from right to left yields the relation to the second branch

$$B_2(k, z) = B_0(k, z) - [\pi/(2 \log \delta e^{i\pi/4} - \log z)]^{\frac{1}{2}}.$$

The choice of this particular principal branch is made to facilitate the study of the branching behavior by means of the operator $\Omega[B]$. To simplify our discussion, let us introduce the variable $\sigma \equiv z + \frac{1}{2}(\zeta + 1/\zeta)(z^2 - 1)^{\frac{1}{2}}$, and hence refer to the mapping $\Omega : B(k, \sigma) \to A(k, z)$.

We wish to study the possibility of branching for the function $A(k, z)$ about the singular point $z_0 = \frac{1}{2}(\delta^2 + \delta^{-2})$, which corresponds to the singular point $\sigma = \delta^2 \neq 1$ of $B(k, \sigma)$. To do this, we consider the following integral, where $\epsilon > 0$ is arbitrarily small,

$$A(k, z_0 + \epsilon e^{2\pi i}) - A(k, z_0 + \epsilon)$$

$$\equiv \int_0^{2\pi} \frac{\partial A}{\partial z_0}(k, z_0 + \epsilon e^{i\theta})\, d\theta$$

$$= \frac{1}{2\pi i} \int_0^{2\pi} d\theta \left\{ \int_{|\zeta|=1} \frac{\partial B(k, \sigma)}{\partial \sigma} \frac{\partial \sigma}{\partial \theta} \frac{d\zeta}{\zeta} \right\}. \qquad (21)$$

If the integrand is absolutely integrable on the product space $\{|\zeta| = 1\} \times \{0 \leq \theta \leq 2\pi\}$, then we may interchange orders of integration. This is certainly satisfied if $B(k, \sigma)$ is $O([\sigma - \delta^2]^{-\alpha})$, $\alpha < 1$, about $\sigma = \delta^2$, which can be shown to be true by the method of dominants.

We consider the mapping $z \to \sigma$ for fixed ζ. Then the circle $|z - z_0| = \epsilon$ is mapped onto the closed curve

[17] See Vol. I of Ref. 10, pp. 27–31.
[18] See Ref. 10, p. 31.

$$C_\phi \equiv \Big\{\sigma \mid \sigma \approx z_0 + (z_0^2 - 1)^{\frac{1}{2}} \cos\phi + \epsilon\Big[e^{i\theta} + \frac{z_0}{(z_0^2 - 1)^{\frac{1}{2}}} \cos\phi\Big]; 0 \leq \theta \leq 2\pi\Big\},$$

where $\phi = \arg \zeta$; the integral (21) becomes

$$A(k, z_0 + \epsilon e^{2\pi i}) - A(k, z_0 + \epsilon) = \frac{1}{2\pi} \int_0^{2\pi} d\phi \int_{C_\phi} \frac{\partial B}{\partial \sigma}\, d\sigma.$$

Since $z_0 + (z_0^2 + 1)^{\frac{1}{2}} = \delta^2$, we may rewrite our expression for C_ϕ as

$$\sigma - \delta^2 = -(1 - \cos\phi)(z_0^2 - 1)^{\frac{1}{2}} + \epsilon\Big[e^{i\theta} + \frac{z_0}{(z_0^2 - 1)^{\frac{1}{2}}} \cos\phi\Big] + O(\epsilon^2),$$

where $\theta \in [0, 2\pi]$. We now subdivide the ϕ interval from 0 to 2π into three parts $[0, \phi_1)$, (ϕ_1, ϕ_2), and $(\phi_2, 2\pi]$, where $\phi_1 < \phi_2$ are roots of the equation ($z_0 \neq 0, 1$)

$$\cos\phi = 1 + \frac{\epsilon}{(z_0^2 - 1)^{\frac{1}{2}}}\Big[1 + \frac{z_0}{(z_0^2 - 1)^{\frac{1}{2}}}\Big] + O(\epsilon^2).$$

It is clear if $\phi \in [0, \phi_1)$ or $(\phi_2, 2\pi]$ that the curve C_ϕ winds about the point $\sigma = \delta^2$ exactly once; whereas, for $\phi \in (\phi_1, \phi_2)$, C_ϕ does not contain $\sigma = \delta^2$. Hence, we may rewrite (making use of symmetry) integral (21) as

$$\begin{aligned} A(k, z + \epsilon e^{2\pi i} - A(k, z + \epsilon) &= \frac{1}{2\pi} \int_0^{\phi_1} d\phi + \int_{\phi_1}^{2\pi} d\phi \Big\{\int_{C_\phi} \frac{\partial B(k, \sigma)}{\partial \sigma}\, d\sigma\Big\} \\ &= \frac{1}{\pi} \int_0^{\phi_1} d\phi\, \{B_2(k, z[\phi]) - B_0(k, z[\phi])\} \\ &= \frac{1}{\pi^{\frac{1}{2}}} \int_0^{\phi_1} \Big\{-\log \frac{z[\phi]}{\delta^2 e^{\frac{1}{2}i\pi}}\Big\}^{-\frac{1}{2}} d\phi, \end{aligned}$$

where

$$z[\phi] = z_0 + (z_0^2 - 1)^{\frac{1}{2}} \cos\phi + \epsilon\Big[1 + \frac{z_0}{(z_0^2 - 1)^{\frac{1}{2}}} \cos\phi\Big] + O(\epsilon^2). \tag{22}$$

We note that the point $z[\phi]$, the intersection point of C_ϕ with the cut $\sigma = \delta^2 + i\lambda$, $\lambda \geq 0$, is a monotone decreasing function for $\phi \in [0, \phi_1)$; hence, our last integral does not vanish. We conclude from this that the difference, $A(k, z + \epsilon e^{2\pi i}) - A(k, z + \epsilon) \neq 0$, and $A(k, z)$ is not single valued in a neighborhood of $z = \frac{1}{2}(\delta^2 + \delta^{-2})$.

Summarizing our results above along with those obtained by considering the determinants $D_i^{(r)}$, we have the following theorem.

Theorem 1: The scattering amplitude $A(k, z)$ which corresponds to a superposition of Yukawa potentials is multiple valued about the singularity at the point $z = (1 + \mu_0^2/4k^2)^{\frac{1}{2}}$, which, moreover, cannot be a polelike branch point. The discontinuity across the branch cut (originating at this singularity), $z = (1 + \mu_0^2/4k^2)^{\frac{1}{2}} + i\lambda$, $\lambda \geq 0$, is given by expression (22).

The results of the above discussion may be generalized in an obvious manner to yield a new method for studying the branching of scattering amplitudes, $A(k, z)$, about a singularity.

Theorem 2: Let the associated function $B(k, \sigma)$ have an isolated singularity at $\sigma = \alpha$, but be regular in the disk $|\sigma| < |\alpha|$. Furthermore, let $B(k, \sigma)$ be majorized by $(\sigma - \alpha)^{-\mu}$, $\mu < +1$, in a neighborhood of α. Finally, let the difference of the value of the principal branch, $B_0(k, \sigma)$, and the branch $B_2(k, \sigma)$, obtained by passing over the cut $\Lambda \equiv \{\sigma \mid \sigma = \alpha + i\lambda, \lambda \geq 0\}$ from right to left, be given by

$$B_2(k, \sigma) - B_0(k, \sigma) = \Delta B(k, \sigma).$$

Then, the corresponding scattering amplitude $A(k, z)$ is single valued about $z_0 = \frac{1}{2}(\alpha + 1/\alpha)$, whenever the following integral vanishes.

$$A(k, z + \epsilon e^{2\pi i}) - A(k, z + \epsilon) = \frac{1}{\pi} \int_0^{\phi_1} \Delta B(k, z[\phi])\, d\phi,$$

with

$$z[\phi] = z_0 + (z_0^2 - 1)^{\frac{1}{2}} \cos\phi + \epsilon\Big[1 + \frac{z_0}{(z_0^2 - 1)^{\frac{1}{2}}} \cos\phi\Big] + O(\epsilon^2),$$

for $\epsilon > 0$ arbitrarily small, and ϕ_1 the smallest positive root of

$$\cos\phi = 1 + \frac{\epsilon}{(z_0^2 - 1)^{\frac{1}{2}}}\Big[1 + \frac{z_0}{(z_0^2 - 1)^{\frac{1}{2}}}\Big] + O(\epsilon^2).$$

A natural question that arises in our study of the singularities of $A(k, z)$ is what type of singularity of $B(k, z)$ corresponds to a pole in the z plane of $A(k, z)$. To answer this question we return to our integral operators $\Omega[B]$ and $\Omega^{-1}[A]$. Let us consider the case where

$$A(k, \xi) \equiv [(\xi - \alpha[k])^m]^{-1} + \text{entire function}.$$

Since no loss of generality occurs by assuming $m = 1$ (as we shall see), we consider those $B(k, z)$ defined by

$$B(k, z) = \Omega^{-1}[(\xi - \alpha[k])^{-1}].$$

The entire part of $A(k, z)$ does not lead to finite singularities, and hence may be ignored. This leads us to evaluate[19]

$$B(k,z) = \frac{1-z^2}{2}\int_{-1}^{+1}\frac{d\xi}{(\xi-\alpha[k])(1-2\xi z+z^2)^{\frac{1}{2}}}$$

$$= \frac{1-z^2}{(z^2-2z\alpha+1)}\left[\frac{1}{(z^2-2\xi z+1)^{\frac{1}{2}}}\right]_{\xi=-1}^{+1}$$

$$+\frac{1-z^2}{2(z^2-2z\alpha+1)^{\frac{1}{2}}}\left\{\log\left[C_1\frac{(z^2-2\xi z+1)^{\frac{1}{2}}-(z^2-2z\alpha+1)^{\frac{1}{2}}}{(z^2-2\xi z+1)^{\frac{1}{2}}+(z^2-2z\alpha+1)^{\frac{1}{2}}}\right]\right\}_{\xi=-1}^{+1}$$

$$= \frac{-2}{z^2-2z\alpha+1}+\frac{\frac{1}{2}(1-z^2)}{(z^2-2z\alpha+1)^{\frac{1}{2}}}\log\left[\frac{1+z\alpha+(z^2-2z\alpha+1)^{\frac{1}{2}}}{1+z\alpha-(z^2-2z\alpha+1)^{\frac{1}{2}}}\right].$$

Hence, for z in a neighborhood of $z_0 = \frac{1}{2}(\alpha + 1/\alpha)$, $B(k, z)$ has the expansion,

$$B(k,z) = \frac{1}{z\alpha-1}+(1-z^2)\times\sum_{m=0}^{\infty}\frac{(z^2-2\alpha z+1)^m}{(2m+3)(1-z\alpha)^{2m+3}},$$

which is clearly analytic regular. We conclude that there do not exist any polar singularities for scattering amplitudes of the form given above. In a similar way, we may discuss the case where $A(k, z)$ has a pole of order m by writing

$$B(k,z) = \Omega^{-1}\left[\frac{1}{(\xi-\alpha)^m}\right] = (m-1)!\frac{\partial^{m-1}}{\partial\alpha^{m-1}}\Omega^{-1}\left[\frac{1}{\xi-\alpha}\right].$$

We list this result as Theorem 3.

Theorem 3: There are no scattering amplitudes that have polar singularities of the form

$$A(k,z) = \sum_{i=1}^{N}\frac{1}{(z-\alpha_i[k])^{m_i}} + \text{entire function}.$$

We conclude this work by listing several theorems which are analogous to those obtained by Gilbert[20] in an earlier study of a certain partial differential equation.

Theorem 4: Let $A_1(k, z)$ and $A_2(k, z)$ be two scattering amplitudes defined by the series expansions,

$$A_\nu(k,z) = \sum_{l=0}^{\infty}a_l^{(\nu)}(k)P_l(z) \qquad (\nu = 1, 2).$$

Furthermore, let us suppose that $A_\nu(k, z)$ $(\nu = 1, 2)$ is singular for

$$z + \tfrac{1}{2}[\alpha_\nu[k] + (\alpha_\nu[k])^{-1}] \qquad (\nu = 1, 2).$$

Then the scattering amplitude given by

$$A_3(k,z) = \sum_{l=0}^{\infty}a_l^{(1)}(k)a_l^{(2)}P_l(z)$$

is singular for $z = \frac{1}{2}[(\alpha_1[k]\alpha_2[k]) + (\alpha_1[k]\alpha_2[k])^{-1}]$.

Theorem 5: Let $A(k, z)$ be a scattering amplitude with the partial wave expansion,

$$A(k,z) = \sum_{l=0}^{\infty}a_l(k)P_l(z),$$

where for each $k \in \mathfrak{D} \subset \mathbf{C}^{(1)}$ one has $\overline{\lim}_{l\to\infty}|a_l(k)|^{1/l} = 0$. Furthermore, if

$$\lambda = \overline{\lim_{l\to\infty}}\frac{l\log l}{\log 1/|a_l(k)|},$$

then in the region $\mathfrak{D} \times \{z \mid |z|^2 + |z^2 - 1| \leq R\}$, $A(k, z)$ satisfies the inequality

$$|A(k,z)| \leq \exp(R^{\lambda+\epsilon})$$

for R sufficiently large and arbitrary $\epsilon > 0$.

The proof is analogous to that of Gilbert.[21] We remark in conclusion that Khuri[22,23] has also studied the analytic properties of the Legendre series (2). His approach, however, differs from ours in that he rearranges (2) to become a power series in the variable z. Since the Legendre polynomials may be approximated asymptotically[24] as $l \to \infty$ by

$$P_n(z) \approx (2\pi n)^{-\frac{1}{2}}(z^2-1)^{-\frac{1}{4}}\{z+(z^2-1)^{\frac{1}{2}}\}^{n+\frac{1}{2}},$$

it is apparent that these two approaches should lead to some similar results.

[19] W. Gröbner and N. Hofreiter, *Unbestimmte Integrale* (Springer-Verlag, Wien, 1949).
[20] See Ref. 14.
[21] See Ref. 14, p. 991.
[22] N. Khuri, Phys. Rev. **132**, 914 (1963).
[23] N. Khuri, Phys. Rev. Letters **10**, 420 (1963).
[24] G. Szegö, *Orthogonal Polynomials* (Colloquium Publications, American Mathematical Society, Providence, R. I., 1939), Vol. 23.

Variational Principle for Eigenvalue Equations

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A variational principle is developed to provide an estimate of an arbitrary functional of the eigenfunctions of a set of eigenvalue equations. It is shown that the variational formalism is equivalent to a functional Taylor series expansion of the desired functional about the trial functions. The relationship of this work to perturbation theory is considered, and it is shown that the formalism can be used to construct higher-order variational principles, i.e., those for which first-order errors in the trial functions leads to an nth-order error in the desired functional. Finally, it is shown that the variational principle of Borowitz and Vassell for estimating off-diagonal matrix elements, as well as the usual Rayleigh quotient, are special cases of the principle presented here.

I. INTRODUCTION

VARIATIONAL methods have found widespread use in mathematical physics. In particular, the Rayleigh quotient[1] is often used for estimating eigenvalues, and the Schwinger variational principle[2] can be used to estimate an arbitrary linear functional of the solution to an inhomogeneous equation. It can be shown[3] that both of these variational principles can be derived from the more basic Roussopoulos principle.[4] Recently, two papers have appeared which generalize the Roussopoulos principle for inhomogeneous equations. The first of these, by Kostin and Brooks,[5] gives two nth-order principles for linear functionals. That is, these principles have the characteristic that first-order errors in the trial functions (actually trial operators) lead to nth-order errors in the estimate of the desired linear functional. The second paper,[6] by the present author, generalizes the Roussopoulos formalism to provide an estimate of an arbitrary (not necessarily linear) functional of the solution to an inhomogeneous equation, with first-order errors in the trial functions leading to second-order errors in the estimate. A generalization of the Schwinger method to provide an estimate of an arbitrary functional of the solution to an inhomogeneous equation is also presented in that paper.

In this paper we present a variational principle for a set of eigenvalue equations which allows one to estimate an arbitrary functional of the eigenfunctions of these equations. The principle is constructed along the lines previously used by the author for inhomogeneous equations.[6] We show the connection of this variational method to a functional Taylor series expansion of the desired functional about the trial functions. We also show the relationship of this work to perturbation theory and how the formalism can be used to construct higher-order principles, analogous to those of Kostin and Brooks[5] for estimating linear functionals of the solution to an inhomogeneous problem. Finally, we show that the variational principle of Borowitz and Vassell[7] for estimating off-diagonal matrix elements, as well as the usual Rayleigh quotient for estimating eigenvalues, are special cases of the principle presented here. Borowitz and Gerjuoy[8] have recently outlined a general procedure for deriving variational principles for estimating an arbitrary functional of the solution to the time-independent Schrödinger equation. Although their considerations are quite different from those of this paper, the results of the two approaches are identical in the two cases (diagonal and off-diagonal matrix elements) to which they applied their procedure.

II. PRINCIPLE FOR A SINGLE EQUATION

We consider the eigenvalue equation,

$$A(x)\psi_i(x) = \Lambda_i B(x)\psi_i(x), \tag{1}$$

where x is the independent variable (or represents the set of independent variables), $\psi_i(x)$ is the jth

[1] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), p. 1108.
[2] H. Levine and J. Schwinger, Phys. Rev. **75**, 1423 (1949).
[3] D. S. Selengut, Hanford Laboratories Report HW-59126 (1959).
[4] P. Roussopoulos, Compt. Rend. **236**, 1858 (1953).
[5] M. D. Kostin and H. Brooks, J. Math. Phys. **5**, 1691 (1964).
[6] G. C. Pomraning, J. Soc. Indust. Appl. Math. **13**, 511 (1965).
[7] S. Borowitz and M. O. Vassell, J. Quant. Spectry. & Radiative Transfer **4**, 663 (1964).
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eigenfunction, Λ_j is the jth eigenvalue, and $A(x)$ and $B(x)$ are real, but not necessarily self-adjoint (Hermitian), operators. The eigenvalues Λ_j are assumed real and nondegenerate. In certain applications, such as quantum mechanics, the special case $B(x) = 1$ and $A(x)$ a self-adjoint operator, is of particular interest. It should also be emphasized that since we have assumed discrete eigenvalues, the application to quantum mechanics of the formalism in the form given in this paper is only valid for bound states. Associated with Eq. (1) is the adjoint equation which has the same eigenvalues, i.e.,

$$A^*(x)\psi_j^*(x) = \Lambda_j B^*(x)\psi_j^*(x), \tag{2}$$

where $A^*(x)$ and $B^*(x)$ are the operators adjoint to $A(x)$ and $B(x)$ according to the usual definition. The functions $\psi_j(x)$ and $\psi_j^*(x)$ form a biorthogonal set with respect to the operator $B(x)$, i.e.,

$$\int dx\ \psi_i^*(x)B(x)\psi_j(x) = \int dx\ \psi_j(x)B^*(x)\psi_i^*(x) = 0, \qquad i \neq j. \tag{3}$$

We wish to construct a variational expression to estimate $G[\psi_j(x)]$, an arbitrary homogeneous functional of $\psi_j(x)$. A homogeneous functional is defined as one which satisfies

$$G[\psi_j(x)] = G[\alpha\psi_j(x)], \tag{4}$$

where α is an arbitrary constant. It is clear that only homogeneous functionals can be of interest since Eq. (1) is homogeneous.

We consider the functional

$$F[\varphi_j(x), \theta_j(x), \lambda_j] = G[\varphi_j(x)] + \int dx\ \theta_j(x)[A(x)\varphi_j(x) - \lambda_j B(x)\varphi_j(x)], \tag{5}$$

where $\varphi_j(x)$ and λ_j are estimates of the jth eigenfunction and eigenvalue, respectively, and are assumed to differ from the exact quantities by first-order terms, i.e.,

$$\varphi_j(x) = \psi_j(x) + \delta\varphi_j(x), \tag{6}$$

$$\lambda_j = \Lambda_j + \delta\lambda_j. \tag{7}$$

Likewise, $\theta_j(x)$ is taken to be a first-order estimate of $\chi_j(x)$ which satisfies an, as yet unspecified, auxiliary equation, i.e.,

$$\theta_j(x) = \chi_j(x) + \delta\theta_j(x). \tag{8}$$

Equation (5) can be thought of as arising in the following way: We wish to compute a stationary estimate of $G[\psi_j(x)]$ subject to the conditions imposed by Eq. (1). These conditions can be incorporated by the standard Lagrange multiplier technique with $\theta_j(x)$ being this multiplier. Since Eq. (1) holds for all x, the sum of the conditions implied by Eq. (1) takes the form of an integral in Eq. (5).

To prove that $F[\varphi_j(x), \theta_j(x), \lambda_j]$ is actually a variational estimate of $G[\psi_j(x)]$, we must show

$$F[\psi_j(x), \chi_j(x), \Lambda_j] = G[\psi_j(x)], \tag{9}$$

$$\delta F[\psi_j(x), \chi_j(x), \Lambda_j] = 0. \tag{10}$$

That is, we must first show that the functional F yields the exact result for $G[\psi_j(x)]$ if the exact solutions of the eigenvalue and auxiliary problems are used, and secondly that first-order errors in these solutions give rise to second-order errors in the estimate. The first condition, Eq. (9), is immediately evident by virtue of Eq. (1). We force Eq. (10) to be satisfied by properly choosing the auxiliary problem. The first variation of Eq. (5) is

$$\begin{aligned}\delta F[\varphi_j(x), \theta_j(x), \lambda_j] &= \int dx\ \delta\theta_j(x)[A(x)\varphi_j(x) - \lambda_j B(x)\varphi_j(x)] \\ &\quad - \delta\lambda_j \int dx\ \theta_j(x)B(x)\varphi_j(x) \\ &\quad + \int dx\ \delta\varphi_j(x)\{A^*(x)\theta_j(x) \\ &\quad - \lambda_j B^*(x)\theta_j(x) + G'[\varphi_j(\xi); x]\}.\end{aligned} \tag{11}$$

$G'[\varphi_j(\xi); x]$ in Eq. (11) denotes the first functional derivative of $G[\varphi_j(x)]$ and is formally given by[9]

$$G'[\varphi(\xi); x] \equiv \lim_{\epsilon \to 0}\left\{\frac{G[\varphi(\xi) + \epsilon\delta(x - \xi)] - G[\varphi(\xi)]}{\epsilon}\right\}, \tag{12}$$

where $\delta(x)$ is the Dirac delta function. Evaluating Eq. (11) with $\psi_j(x)$ and Λ_j, we see that the first term on the right-hand side vanishes. The last term can be made to vanish when $\varphi_j(x) = \psi_j(x)$ and $\lambda_j = \Lambda_j$ if $\chi_j(x)$, to which $\theta_j(x)$ is a first-order approximation, satisfies

$$A^*(x)\chi_j(x) - \Lambda_j B^*(x)\chi_j(x) = -G'[\psi_j(\xi); x]. \tag{13}$$

Equation (13) has the form of an eigenvalue problem with an inhomogeneous term. A necessary condition for a problem of this type to have a solution is that the eigenfunction expansion, in the $\psi_i^*(x)$, of

[9] V. Volterra, *Theory of Functionals and of Integral and Integro-Differential Equations* (Dover Publications, Inc., New York, 1959).

the inhomogeneous term have no $i = j$ contribution. In physical terms, we must not drive the system which Eq. (13) describes at its resonant frequency. Because of the biorthogonality condition of the eigenfunctions, the above condition is equivalent to

$$\int dx\ \psi_i(x)G'[\psi_i(\xi);x] = 0. \tag{14}$$

Equation (14) is just a basic property of homogeneous functionals,[9] which is the only class of functionals of interest for the eigenvalue problem.

Finally, we must show that the term involving $\delta\lambda_i$ in Eq. (11) is of second order. If one obtains the trial quantity λ_i from the Rayleigh quotient, i.e.,

$$\lambda_i = \frac{\int dx\ \varphi_i^*(x)A(x)\varphi_i(x)}{\int dx\ \varphi_i^*(x)B(x)\varphi_i(x)}, \tag{15}$$

where $\varphi_i^*(x)$ is a first-order approximation to $\psi_i^*(x)$, then $\delta\lambda_i$ itself is of second order, and we need not investigate the coefficient of $\delta\lambda_i$ in Eq. (11). More generally, however, we can allow first-order errors in λ_i if we choose a particular solution of Eq. (13) for $\chi_i(x)$. With the assumption that the eigenfunctions defined by Eq. (2) form a complete set, a solution for $\chi_i(x)$ is

$$\chi_i(x) = \sum_{i\neq j}\left[\frac{\alpha_{ij}}{\Lambda_j - \Lambda_i}\right]\psi_j^*(x), \tag{16}$$

where we have defined

$$\alpha_{ij} \equiv \frac{\int dx\ G'[\psi_i(\xi);x]\psi_i(x)}{\int dx\ \psi_i(x)B^*(x)\psi_j^*(x)}. \tag{17}$$

Because of the biorthogonality condition of the eigenfunctions, we have, with $\chi_i(x)$ given by Eq. (16),

$$\int dx\ \chi_i(x)B(x)\psi_i(x) = 0, \tag{18}$$

and hence the coefficient of $\delta\lambda_i$ in Eq. (11) is of first order, making the product of this coefficient and a first-order $\delta\lambda_j$ a second-order quantity.

However, if one allows a first-order $\delta\lambda_j$, care must be taken to ensure that $\theta_i(x)$ is a first-order approximation to $\chi_i(x)$ as given by Eq. (16), which is only a particular solution of Eq. (13). The general solution of Eq. (13), which we denote by $\chi_i'(x)$ to distinguish it from Eq. (16), is

$$\chi_i'(x) = \sum_{i\neq j}\left[\frac{\alpha_{ij}}{\Lambda_j - \Lambda_i}\right]\psi_j^*(x) + \Gamma\psi_i^*(x), \tag{19}$$

where Γ is an arbitrary constant. A first-order approximation to $\chi_i'(x)$, with Γ other than zero (or a first-order quantity), coupled with a first-order $\delta\lambda_j$, yield a first-order, rather than a second-order, δF and the functional given by Eq. (5) yield an estimate of $G[\psi_i(x)]$ which is no more accurate, in general, than $G[\varphi_i(x)]$, obtained from a direct calculation with the trial function, $\varphi_i(x)$. However, in practice this offers no great difficulty. If one finds an arbitrary solution to Eq. (13), i.e., Eq. (19), one can easily construct from this the proper solution to use in connection with a first-order $\delta\lambda_i$, i.e., Eq. (16). We have

$$\chi_i(x) = \chi_i'(x) - \frac{\psi_i^*(x)\int d\xi\ \psi_i(\xi)B^*(\xi)\chi_i'(\xi)}{\int d\xi\ \psi_i(\xi)B^*(\xi)\psi_i^*(\xi)}. \tag{20}$$

We shortly give the more useful analog of Eq. (20) for $\theta_i'(x)$ and $\theta_i(x)$. That is, if one has a first-order approximation to $\chi_i'(x)$, given by Eq. (19), we show how one easily constructs a first-order approximation to $\chi_i(x)$, given by Eq. (16), which is the required trial function in connection with a first-order $\delta\lambda_i$.

To summarize, we have shown that if $\varphi_i(x)$ is a first-order approximation to $\psi_i(x)$, if λ_i is a first-order approximation to Λ_i, and if $\theta_i(x)$ is a first-order approximation to $\chi_i(x)$ as given by Eq. (16), then the functional given by Eq. (5) yields an estimate of $G[\psi_i(x)]$ containing only second-order errors in $\delta\varphi_i(x)$, $\delta\theta_i(x)$, and $\delta\lambda_i$.

We note that the defining equation for $\chi_i(x)$, Eq. (13), depends upon the exact solution of the eigenvalue problem, $\psi_i(x)$ and Λ_i, which by hypothesis is not known. This is not particularly disturbing since we do not require an exact solution of Eq. (13). We need only a first-order approximation to $\chi_i(x)$. Nevertheless, it seems desirable to replace Eq. (13) with an equation for $\bar{\chi}_i(x)$, which differs from $\chi_i(x)$ by first-order terms, and which contains no reference to the exact eigenfunction, $\psi_i(x)$, or the exact eigenvalue, Λ_i. One such equation is

$$A^*(x)\bar{\chi}_i(x) - \lambda_i B^*(x)\beta_i(x)\bar{\chi}_i(x) = -G'[\varphi_i(\xi);x], \tag{21}$$

where we have defined

$$\beta_i(x) \equiv A(x)\varphi_i(x)/\lambda_i B(x)\varphi_i(x). \tag{22}$$

We can easily demonstrate that the solutions for $\chi_i(x)$ and $\bar{\chi}_i(x)$ needed in connection with a first-order $\delta\lambda_i$ differ by first-order terms only. For this purpose we define the eigenfunctions $\bar{\psi}_{ij}^*(x)$ and eigenvalues $\bar{\Lambda}_{ij}$ by

$$A^*(x)\bar{\psi}_{ij}^*(x) = \bar{\Lambda}_{ij}B^*(x)\beta_i(x)\bar{\psi}_{ij}^*(x). \tag{23}$$

These eigenfunctions are orthogonal to the set $\bar{\psi}_{ij}(x)$ defined by

$$A(x)\bar{\psi}_{ij}(x) = \bar{\Lambda}_{ij}\beta_i(x)B(x)\bar{\psi}_{ij}(x), \tag{24}$$

with the orthogonality relationship being

$$\int dx\ \bar{\psi}_{i}^{*}(x)\beta_i(x)B(x)\bar{\psi}_{ki}(x)$$

$$= \int dx\ \bar{\psi}_{ki}(x)B^*(x)\beta_i(x)\bar{\psi}_{i}^{*}(x) = 0, \quad i \neq k. \tag{25}$$

In particular, we have

$$\bar{\psi}_{ii}(x) = \varphi_i(x), \tag{26}$$

$$\bar{\Lambda}_{ii} = \lambda_i. \tag{27}$$

A particular solution to Eq. (21) is then given by

$$\tilde{\chi}_i(x) = \sum_{i \neq j} \left[\frac{\bar{\alpha}_{ij}}{\lambda_i - \bar{\Lambda}_{ij}} \right] \bar{\psi}_{i}^{*}(x), \tag{28}$$

where we have defined

$$\bar{\alpha}_{ij} \equiv \frac{\int dx\ G'[\varphi_i(\xi); x]\bar{\psi}_{ij}(x)}{\int dx\ \bar{\psi}_{ij}(x)B^*(x)\beta_i(x)\bar{\psi}_{i}^{*}(x)}. \tag{29}$$

Since $\beta_i(x)$ differs from unity by first-order terms only, it is clear from perturbation theory arguments that $\psi_{i}^{*}(x)$ and $\bar{\psi}_{i}^{*}(x)$, as well as Λ_i and $\bar{\Lambda}_{ij}$, and $\psi_i(x)$ and $\bar{\psi}_{ij}(x)$, differ by first-order terms only. It then follows that α_{ij} and $\bar{\alpha}_{ij}$ differ by first-order terms. Finally, a comparison of the right-hand sides of Eqs. (16) and (28) shows that $\chi_i(x)$ and $\tilde{\chi}_i(x)$ are equal to within first-order terms, as postulated. The general solution of Eq. (21), which we denote by $\tilde{\chi}_i'(x)$, is found by adding the term $\Gamma\bar{\psi}_{i}^{*}(x)$ to the right-hand side of Eq. (28), where Γ is an arbitrary constant. Analogous to Eq. (20), we have the connection formula

$$\tilde{\chi}_i(x) = \tilde{\chi}_i'(x) - \frac{\bar{\psi}_{i}^{*}(x) \int d\xi\ \varphi_i(\xi)B^*(\xi)\beta_i(\xi)\tilde{\chi}_i'(\xi)}{\int d\xi\ \varphi_i(\xi)B^*(\xi)\beta_i(\xi)\bar{\psi}_{i}^{*}(\xi)}. \tag{30}$$

Unfortunately, $\bar{\psi}_{i}^{*}(x)$ is not related to the trial functions $\varphi_i(x)$ or $\varphi_{i}^{*}(x)$ in any simple manner as is $\bar{\psi}_{ij}(x)$ [see Eq. (26)], but it can be shown that $\bar{\psi}_{i}^{*}(x)$ and $\varphi_{i}^{*}(x)$ differ by first-order terms only.

Hence $\theta_i(x)$, needed in Eq. (5), can be taken as a first-order approximation to either $\chi_i(x)$ given by Eq. (16) or $\tilde{\chi}_i(x)$ given by Eq. (28). In practice it may be easier to obtain $\theta_i(x)$ as an approximation to $\tilde{\chi}_i(x)$ since the defining equation for $\tilde{\chi}_i(x)$ contains only the known quantities, $A(x)$, $A^*(x)$, $B(x)$, $B^*(x)$, and $\varphi_i(x)$. To complete the argument, one final practical point needs discussion. If one obtains a function $\theta_i'(x)$, a first-order approximation to an arbitrary solution of either Eq. (13) or Eq. (21), how does one obtain the function $\theta_i(x)$ needed as the trial function for use with a first-order $\delta\lambda_i$? It is easily shown that $\theta_i(x)$ defined by

$$\theta_i(x) = \theta_i'(x) - \frac{\varphi_{i}^{*}(x) \int d\xi\ \varphi_i(\xi)B^*(\xi)\beta_i(\xi)\theta_i'(\xi)}{\int d\xi\ \varphi_i(\xi)B^*(\xi)\beta_i(\xi)\theta_{i}^{*}(\xi)}, \tag{31}$$

or equivalently, to first order,

$$\theta_i(x) = \theta_i'(x) - \frac{\varphi_{i}^{*}(x) \int d\xi\ \varphi_i(\xi)B^*(\xi)\theta_i'(\xi)}{\int d\xi\ \varphi_i(\xi)B^*(\xi)\varphi_{i}^{*}(\xi)}, \tag{32}$$

differs from Eqs. (16) and (28) by first-order quantities and, hence, is the desired trial function. It should be re-emphasized that if one uses the Rayleigh quotient Eq. (15) to obtain λ_i, then $\delta\lambda_i$ is of second order and $\theta_i'(x)$ can be used directly as the trial function without first modifying it according to Eq. (31) or Eq. (32).

III. RELATIONSHIP TO OTHER WORK

In this section we relate our variational principle to other mathematical techniques. For simplicity, we consider the self-adjoint problem (so that $\psi_i = \psi_{i}^{*}$ and $\varphi_i = \varphi_{i}^{*}$)

$$A(x)\psi_i(x) = \Lambda_i\psi_i(x). \tag{33}$$

We can very easily show the relationship of this variational principle to a functional Taylor series expansion of $G[\psi_i(x)]$ about $G[\varphi_i(x)]$. Using Eqs. (6), (7), and (8) in the integral term of the functional, Eq. (5), and using the defining equations for $\psi_i(x)$, Λ_i, and $\chi_i(x)$, Eqs. (1) and (13), we find

$$F[\varphi_i(x), \theta_i(x), \lambda_i]$$

$$= G[\varphi_i(x)] - \int dx\ \delta\varphi_i(x)G'[\psi_i(\xi); x]$$

$$+ O(\delta\varphi_i\ \delta\theta_i + \delta\lambda_i\ \delta\varphi_i + \delta\lambda_i\ \delta\theta_i), \tag{34}$$

where the symbol $O(\epsilon)$ means "of the order of ϵ." With the assumption that $G'[\psi_i(\xi); x]$ has a functional derivative, Eq. (34) can be rewritten as

$$F[\varphi_i(x), \theta_i(x), \lambda_i]$$

$$= G[\varphi_i(x)] - \int dx\ \delta\varphi_i(x)G'[\varphi_i(\xi); x]$$

$$+ O(\delta\varphi_i\ \delta\theta_i + \delta\lambda_i\ \delta\varphi_i + \delta\lambda_i\ \delta\theta_i + \delta\varphi_i\ \delta\varphi_i). \tag{35}$$

Equation (35) is the desired result and shows the identity, to first order, between the variational result and a functional Taylor series expansion of $G[\psi_i(x)]$ about $G[\varphi_i(x)]$. Equation (35) can also be rewritten

$$F[\varphi_i(x), \theta_i(x), \lambda_i]$$

$$= G[\psi_i(x)] + O(\delta\varphi_i\ \delta\theta_i + \delta\lambda_i\ \delta\varphi_i$$

$$+ \delta\lambda_i\ \delta\theta_i + \delta\varphi_i\ \delta\varphi_i), \tag{36}$$

which explicitly shows the order of the error involved in the variational estimate.

We can just as easily show that the Rayleigh quotient, Eq. (15), is a special case of the principle given in this paper. If we choose the functional $G[\varphi_i(x)]$ to be the Rayleigh quotient, then

$$G'[\varphi_i(\xi); x] = \frac{2A(x)\varphi_i(x)}{\int d\xi[\varphi_i(\xi)]^2} - \frac{2\varphi_i(x)\int d\xi\, \varphi_i(\xi)A(\xi)\varphi_i(\xi)}{\{\int d\xi[\varphi_i(\xi)]^2\}^2}. \tag{37}$$

Evaluating Eq. (37) with the exact eigenfunction, $\psi_i(x)$, we find $G'[\psi_i(\xi); x] = 0$, and thus the auxiliary equation given by Eq. (13) becomes

$$A(x)\chi_i(x) - \Lambda_i\chi_i(x) = 0. \tag{38}$$

Equation (38) has the solution $\chi_i(x) = 0$, and thus we may take $\theta_i(x) = 0$ in the functional, Eq. (5). This yields

$$F[\varphi_i(x)] = G[\varphi_i(x)] = \frac{\int dx\, \varphi_i(x)A(x)\varphi_i(x)}{\int dx[\varphi_i(x)]^2}. \tag{39}$$

We see that we have just recovered the Rayleigh quotient, and we conclude that the Rayleigh quotient is a special case of the more general principle contained in Eq. (5).

For the purpose of relating the variational principle to perturbation theory, we consider the operator in Eq. (33) to be composed of two parts and write

$$A(x) = A_0(x) + A_1(x), \tag{40}$$

where $A_1(x)$ is a small perturbation on $A_0(x)$. If we consider a first-order perturbation theory treatment, we write

$$\psi_i(x) \approx \psi_{i0}(x) + \psi_{i1}(x), \tag{41}$$

$$\Lambda_i \approx \Lambda_{i0} + \Lambda_{i1}, \tag{42}$$

where subscript 1 indicates a small quantity compared to the corresponding quantity with a zero subscript. Perturbation theory then yields the following identities:

$$A_0(x)\psi_{i0}(x) = \Lambda_{i0}\psi_{i0}(x), \tag{43}$$

$$[A_0(x) - \Lambda_{i0}(x)]\psi_{i1}(x) = [\Lambda_{i1} - A_1(x)]\psi_{i0}(x), \tag{44}$$

$$\Lambda_{i1} = \frac{\int dx\, \psi_{i0}(x)A_1(x)\psi_{i0}(x)}{\int dx\, [\psi_{i0}(x)]^2}. \tag{45}$$

Thus the first-order perturbation theory estimate of the functional $G[\psi_i(x)]$ is

$$G[\psi_i(x)] \approx G[\psi_{i0}(x) + \psi_{i1}(x)], \tag{46}$$

or, expanding the right-hand side of Eq. (46) in a first-order functional Taylor series,

$$G[\psi_i(x)] \approx G[\psi_{i0}(x)] + \int dx\, G'[\psi_{i0}(\xi); x]\psi_{i1}(x). \tag{47}$$

Now, the symbolic solution of Eq. (44) for $\psi_{i1}(x)$ is

$$\psi_{i1}(x) = [A_0(x) - \Lambda_{i0}]^{-1} \times [\Lambda_{i1} - A_1(x)]\psi_{i0}(x) + \Gamma\psi_{i0}(x), \tag{48}$$

where Γ is an arbitrary constant. This arbitrary multiple of $\psi_{i0}(x)$ arises as the solution to the homogeneous portion of Eq. (44). The operator $[A_0(x) - \Lambda_{i0}]^{-1}$ is arbitrary to within an additive multiple of the operator C_{i0} defined by

$$C_{i0}f(x) = \psi_{i0}(x)\int d\xi\, f(\xi). \tag{49}$$

However, since we have explicitly included an arbitrary multiple of $\psi_{i0}(x)$ in Eq. (48), we can define $[A_0(x) - \Lambda_{i0}]^{-1}$ as the particular operator which, when operating on a function orthogonal to $\psi_{i0}(x)$ (it is only for these functions that this operator exists) yields a function orthogonal to $\psi_{i0}(x)$. That is,

$$[A_0(x) - \Lambda_{i0}]^{-1}f(x) \equiv \sum_{i\neq j}\psi_{i0}(x)\left[\frac{\int d\xi\, \psi_{i0}(\xi)f(\xi)}{(\Lambda_{i0} - \Lambda_{j0})\int d\xi\, [\psi_{i0}(\xi)]^2}\right]. \tag{50}$$

With this definition of $[A_0(x) - \Lambda_{i0}]^{-1}$, coupled with the facts that it is a self-adjoint operator and $G[\psi_i(x)]$ is a homogeneous functional, it is easily shown that the use of Eq. (48) in Eq. (47) yields

$$G[\psi_i(x)] \approx G[\psi_{i0}(x)] - \int dx\, [A_1(x)\psi_{i0}(x)] \times [A_0(x) - \Lambda_{i0}]^{-1}G'[\psi_{i0}(\xi); x]. \tag{51}$$

Equation (51) is the final result of the first-order perturbation calculation.

We wish to compare this perturbation theory result with that obtained from the variational method using zeroth-order trial functions, i.e.,

$$\varphi_i(x) = \psi_{i0}(x), \tag{52}$$

$$\lambda_i = \Lambda_{i0}. \tag{53}$$

With these trial functions, the variational expression, Eq. (5), becomes

$$F[\psi_{i0}(x), \theta_i(x), \Lambda_{i0}] = G[\psi_{i0}(x)] + \int dx\, \theta_i(x)A_1(x)\psi_{i0}(x). \tag{54}$$

For $\theta_i(x)$, the trial function for $\chi_i(x)$, we take the

zeroth-order approximation to the exact auxiliary equation given by Eq. (13), i.e.,

$$A_0(x)\theta_i(x) - \Lambda_{i0}\theta_i(x) = -G'[\psi_{i0}(\xi); x]. \quad (55)$$

As discussed in some detail in Sec. II, we require, since the trial eigenvalue is in error by first-order terms, the particular solution to Eq. (55) which is orthogonal to $\psi_{i0}(x)$. This is given formally by

$$\theta_i(x) = -[A_0(x) - \Lambda_{i0}(x)]^{-1}G'[\psi_{i0}(\xi); x], \quad (56)$$

where the inverse operator is the same one encountered in the perturbation theory treatment and is given by Eq. (50). Use of Eq. (56) in Eq. (54) yields

$$F[\psi_{i0}(x); \Lambda_{i0}] = G[\psi_{i0}(x)] - \int dx\, [A_1(x)\psi_{i0}(x)][A_0(x) - \Lambda_{i0}]^{-1}G'[\psi_{i0}(\xi); x], \quad (57)$$

which is identical to the first-order perturbation theory result, Eq. (51). Hence we have established a connection between perturbation theory and the variational principle. Hirschfelder *et al.*[10] have shown this same relationship in two special cases, the Rayleigh quotient and a principle for calculating off-diagonal matrix elements. They have also shown, given a variational principle for a functional G, how one can derive a variational principle for $G^{(n)}$, the nth term in a perturbation theory solution for G.

Although we have restricted our attention to the use of zeroth-order perturbation theory results as the trial functions in the variational method, one could also use higher-order results as trial functions. If one used the results of an $(n-1)$th-order perturbation theory solution of Eqs. (1) and (13) as trial functions in Eq. (5), the variational method would yield an estimate of $G[\psi_i(x)]$ with an error of order ϵ^{2n}, where ϵ denotes the order of $A_1(x)$ as compared to $A_0(x)$. This is the essence of the method used by Kostin and Brooks[5] in constructing their functional j_{Bn}. Their variational principle gives an estimate of a linear functional of the solution to an inhomogeneous problem with an error of the order of ϵ^{2n}, where ϵ is the error in the trial operator. (Kostin and Brooks use trial operators rather than trial functions.) This same class of trial functions could be used in the previous work of the present author[6] which gives generalizations of the Rousopoulos[4] and Schwinger[2] methods to allow one to estimate an arbitrary functional of the solution to an inhomogeneous problem. This would lead to a direct generalization of the j_{Bn} functional to one which would estimate, with errors of the order of ϵ^{2n}, an arbitrary functional (not necessarily linear as treated by Kostin and Brooks) of the solution to an inhomogeneous problem. This functional, together with the functional for eigenvalue problems just discussed, would in principle allow one to estimate, with an arbitrarily small error, an arbitrary functional of the solution to either an inhomogeneous or an eigenvalue problem.

An interesting possibility is to use the variational principle to improve upon the eigenfunction itself. For this purpose, we choose

$$G[\psi_i(x)] = \psi_i(x_0)/L[\psi_i(x)], \quad (58)$$

where $L[\psi_i(x)]$ is an appropriate functional of $\psi_i(x)$ so as to make $G[\psi_i(x)]$ a homogeneous functional. For example, one might take

$$L[\psi_i(x)] = \left\{\int dx\, [\psi_i(x)]^2\right\}^{\frac{1}{2}}. \quad (59)$$

Equation (58) has the functional derivative,

$$G'[\psi_i(\xi); x] = \frac{\delta(x - x_0)}{L[\psi_i(\xi)]} - \frac{\psi_i(x_0)L'[\psi_i(\xi); x]}{\{L[\psi_i(\xi)]\}^2}, \quad (60)$$

where $\delta(x)$ is the Dirac delta function. With this choice of $G[\psi_i(x)]$, the variational method gives an estimate, with second-order errors, of the eigenfunction itself, with the functional $L[\psi_i(x)]$ acting as a normalization factor in this estimate. A further possibility is to use the variational principle repeatedly, with the estimate of the eigenfunction from the nth use of the principle used as the trial function for the $(n+1)$th application. With the assumption that this is a convergent process, one can then obtain the eigenfunction to any desired accuracy.

Mathematically, this procedure can be written, from Eq. (5),

$$\frac{\varphi_i^{(n+1)}(x_0)}{L[\varphi_i^{(n+1)}(x)]} = \frac{\varphi_i^{(n)}(x_0)}{L[\varphi_i^{(n)}(x)]} + \int dx\, \theta_i(x)[A(x)\varphi_i^{(n)}(x) - \lambda_i^{(n)}\varphi_i^{(n)}(x)], \quad (61)$$

where $\varphi_i^{(n)}(x)$ is the nth estimate of the eigenfunction with $\varphi_i^{(0)}(x)$ being the initial trial function, $\lambda_i^{(n)}$ is the nth estimate of the eigenvalue which can be calculated from the Rayleigh quotient,

$$\lambda_i^{(n)} = \frac{\int dx\, \varphi_i^{(n)}(x)A(x)\varphi_i^{(n)}(x)}{\int dx\, [\varphi_i^{(n)}(x)]^2}, \quad (62)$$

[10] J. O. Hirschfelder, W. B. Brown, and S. T. Epstein, *Advances in Quantum Chemistry* (Academic Press Inc., New York, 1964), Vol. I, p. 255.

and $\theta_i(x)$ is an approximation to $\chi_i(x)$ which satisfies

$$A(x)\chi_i(x) - \Lambda_i\chi_i(x) = \frac{\psi_i(x_0)L'[\psi_i(\xi);x]}{\{L[\psi_i(\xi)]\}^2} - \frac{\delta(x-x_0)}{L[\psi_i(\xi)]}. \quad (63)$$

Since $\psi_i(x)$, the exact eigenfunction, is not known in Eq. (63), this equation would be replaced in an actual computation with the equation for $\bar{\chi}_i(x)$ based on the initial trial function, $\varphi_i^{(0)}(x)$. From Eqs. (21) and (22) we find

$$\varphi_i^{(0)}(x)A(x)\bar{\chi}_i(x) - \bar{\chi}_i(x)A(x)\varphi_i^{(0)}(x) = \frac{\varphi_i^{(0)}(x)\varphi_i^{(0)}(x_0)L'[\varphi_i^{(0)}(\xi);x]}{\{L[\varphi_i^{(0)}(\xi)]\}^2} - \frac{\varphi_i^{(0)}(x_0)\,\delta(x-x_0)}{L[\varphi_i^{(0)}(\xi)]}. \quad (64)$$

Let us now make an estimate of the error in $\varphi_i^{(n)}(x)$. We assume that $\varphi_i^{(0)}(x)$, the initial trial function, has an error of order ϵ and that $\theta_i(x)$ has an error of order $\bar{\epsilon}$. From Eq. (62) it is clear that $\lambda_i^{(0)}$ has an error of order ϵ^2. Since in practice $\theta_i(x)$ is obtained as an approximation to $\bar{\chi}_i(x)$ which is in error from $\chi_i(x)$ by order ϵ, $\bar{\epsilon}$ is in general of the order of or larger than ϵ. With this observation, the order of the error in $\varphi_i^{(n)}(x)$, which we denote by E_n, is easily computed. From Eq. (36) we see that the $(\delta\varphi_i\delta\theta_i)$ term is dominant, and we have

$$E_{n+1} = \bar{\epsilon}E_n, \quad (65)$$

the solution to which is, subject to the boundary condition $E_0 = \epsilon$,

$$E_n = \epsilon(\bar{\epsilon})^n. \quad (66)$$

This error could be reduced considerably if the error in the auxiliary trial function, $\theta_i(x)$, is reduced at each step in the n-fold process instead of being held constant at order $\bar{\epsilon}$. That is, we could replace Eqs. (61) and (64) by

$$\frac{\varphi_i^{(n+1)}(x_0)}{L[\varphi_i^{(n+1)}(x)]} = \frac{\varphi_i^{(n)}(x_0)}{L[\varphi_i^{(n)}(x)]} + \int dx\; \theta_i^{(n)}(x)[A(x)\varphi_i^{(n)}(x) - \lambda_i^{(n)}\varphi_i^{(n)}(x)], \quad (67)$$

$$\varphi_i^{(n)}(x)A(x)\bar{\chi}_i^{(n)}(x) - \bar{\chi}_i^{(n)}(x)A(x)\varphi_i^{(n)}(x) = \frac{\varphi_i^{(n)}(x)\varphi_i^{(n)}(x_0)L'[\varphi_i^{(n)}(\xi);x]}{\{L[\varphi_i^{(n)}(\xi)]\}^2} - \frac{\varphi_i^{(n)}(x_0)\,\delta(x-x_0)}{L[\varphi_i^{(n)}(\xi)]}, \quad (68)$$

where $\theta_i^{(n)}(x)$ in Eq. (67) is an approximation to $\bar{\chi}_i^{(n)}(x)$ as defined by Eq. (68). Since $\bar{\chi}_i^{(n)}(x)$ is in error, compared to the exact solution $\chi_i(x)$, by the same order as the error in $\varphi_i^{(n)}(x)$, this is the smallest error which one could expect in $\theta_i^{(n)}(x)$. If one achieved this optimum situation, Eq. (36) implies

$$E_{n+1} = E_n^2, \quad (69)$$

which has the solution, subject to the boundary condition $E_0 = \epsilon$, where ϵ here is the order of the error in both $\varphi_i^{(0)}(x)$ and $\theta_i^{(0)}(x)$,

$$E_n = (\epsilon)^{2^n}. \quad (70)$$

In this case E_n decreases very rapidly with increasing n. Once one has the eigenfunction to the desired accuracy, say with an error given by Eq. (66) or Eq. (70), one can then compute an estimate of $G[\psi_i(x)]$ which is in general also in error by only E_n.

At this point we can easily show the relationship of this work to the second functional of Kostin and Brooks[5] which they denote by j_{An}. This functional, which gives an estimate of a linear functional of the solution to an inhomogeneous problem, has the property that first-order errors in the trial operators lead to nth-order errors in the estimate. The connection of j_{An} to the present work is that it can be derived in the manner we have just outlined for the eigenvalue problem. That is, one uses the basic Roussopoulos formalism[4] for inhomogeneous problems and chooses the inhomogeneous term in the auxiliary problem as a delta function $\delta(x - x_0)$, and repeatedly uses the variational method to improve the solution to the problem of interest. Having obtained the solution to nth order, one computes the linear functional of interest with this solution. The final expression for the linear functional involves repeated integrals over approximate Green's functions. If one defines the integral over the Green's function as the operator G of Kostin and Brooks, one finds the functional j_{An}. The repeated use of the variational method as given by Eq. (61) is the analog of j_{An} for eigenvalue equations.

One can repeat most of the analysis of this section for the more general eigenvalue equation given by Eq. (1). The only exception is the Rayleigh quotient. Since the Rayleigh quotient for a non-self-adjoint equation, Eq. (15), is a functional of both $\varphi_i(x)$ and $\varphi_i^*(x)$, we cannot show the relationship of the present work to the Rayleigh quotient for a non-self-adjoint system before considering a generalization of the formalism.

IV. PRINCIPLE FOR A SET OF EQUATIONS

We consider the set of I eigenvalue equations,

$$A^{(i)}(x)\psi_i^{(i)}(x) = \Lambda_i^{(i)}B^{(i)}(x)\psi_i^{(i)}(x) \qquad (1 \le i \le I), \quad (71)$$

where the superscript i refers to the ith equation and the subscript j refers to the jth eigenfunction. As before, $A^{(i)}(x)$ and $B^{(i)}(x)$ are real, but not necessarily self-adjoint, operators and the eigenvalues $\Lambda_i^{(i)}$ are assumed real, and for a given i, nondegenerate. We wish to estimate the functional $G[\psi_i^{(1)}, \psi_i^{(2)}, \cdots \psi_i^{(I)}]$ which is homogeneous with respect to each function $\psi_i^{(i)}(x)$. For this purpose we consider the functional

$$F[\varphi_i^{(s)}(x), \theta_i^{(s)}(x), \lambda_i^{(s)}] = G[\varphi_i^{(s)}(x)] + \sum_{i=1}^{I} \int dx\ \theta_i^{(i)}(x) \times [A^{(i)}(x)\varphi_i^{(i)}(x) - \lambda_i^{(i)}B^{(i)}(x)\varphi_i^{(i)}(x)], \quad (72)$$

where $\varphi_i^{(i)}(x)$, $\lambda_i^{(i)}$, and $\theta_i^{(i)}(x)$ are first-order approximations to $\psi_i^{(i)}(x)$, $\Lambda_i^{(i)}$, and $\chi_i^{(i)}(x)$, respectively. $\chi_i^{(i)}(x)$ is defined shortly. To simplify the writing in Eq. (72), we have used the superscript s to indicate all of the I quantities in the argument list, i.e.,

$$F[\varphi_i^{(s)}, \theta_i^{(s)}, \lambda_i^{(s)}] \equiv F[\varphi_i^{(1)}, \cdots, \varphi_i^{(I)}, \theta_i^{(1)}, \cdots, \theta_i^{(I)}, \lambda_i^{(1)}, \cdots, \lambda_i^{(I)}], \quad (73)$$

$$G[\varphi_i^{(s)}] \equiv G[\varphi_i^{(1)}, \cdots, \varphi_i^{(I)}]. \quad (74)$$

Clearly, $F[\varphi_i^{(s)}(x), \theta_i^{(s)}(x), \lambda_i^{(s)}]$ reduces to $G[\psi_i^{(s)}(x)]$ if the exact solutions of the I equations given by Eq. (71) are used for $\varphi_i^{(i)}(x)$ and $\lambda_i^{(i)}$. The first variation of Eq. (72) is given by

$$\delta F[\varphi_i^{(s)}(x), \theta_i^{(s)}(x), \lambda_i^{(s)}] = -\sum_{i=1}^{I} \delta\lambda_i^{(i)} \int dx\ \theta_i^{(i)}(x)B^{(i)}(x)\varphi_i^{(i)}(x) + \sum_{i=1}^{I} \int dx\ \delta\theta_i^{(i)}(x) \times [A^{(i)}(x)\varphi_i^{(i)}(x) - \lambda_i^{(i)}B^{(i)}(x)\varphi_i^{(i)}(x)] + \sum_{i=1}^{I} \int dx\ \delta\varphi_i^{(i)}(x)\left\{A^{(i)*}(x)\theta_i^{(i)}(x) - \lambda_i^{(i)}B^{(i)*}(x)\theta_i^{(i)}(x) + \frac{\delta G[\varphi_i^{(s)}(\xi); x]}{\delta\varphi_i^{(i)}}\right\}, \quad (75)$$

where $A^{(i)*}(x)$ and $B^{(i)*}(x)$ are the operators adjoint to $A^{(i)}(x)$ and $B^{(i)}(x)$ and $\delta G[\varphi_i^{(s)}(\xi); x]/\delta\varphi_i^{(i)}$ denotes the first functional derivative of $G[\varphi_i^{(s)}(x)]$ with respect to $\varphi_i^{(i)}(x)$. Following the methods previously used for a single eigenvalue equation, we can show δF to be a second-order quantity if $\varphi_i^{(i)}(x)$ is a first-order approximation to $\psi_i^{(i)}(x)$, $\lambda_i^{(i)}$ is a first-order approximation to $\Lambda_i^{(i)}$, and $\theta_i^{(i)}(x)$ is a first-order approximation to a particular solution for $\chi_i^{(i)}(x)$, defined by

$$A^{(i)*}(x)\chi_i^{(i)}(x) - \Lambda_i^{(i)}B^{(i)*}(x)\chi_i^{(i)}(x) = -\delta G[\psi_i^{(s)}(\xi); x]/\delta\psi_i^{(i)}. \quad (76)$$

It can also be shown, following the methods previously used, that this particular solution for $\chi_i^{(i)}(x)$ differs from a particular solution for $\tilde{\chi}_i^{(i)}(x)$ by first-order terms only if we define $\tilde{\chi}_i^{(i)}(x)$ by the equation

$$A^{(i)*}(x)\tilde{\chi}_i^{(i)}(x) - \lambda_i^{(i)}B^{(i)*}(x)\beta_i^{(i)}(x)\tilde{\chi}_i^{(i)}(x) = -\delta G[\varphi_i^{(s)}(\xi); x]/\delta\varphi_i^{(i)}, \quad (77)$$

where we have defined

$$\beta_i^{(i)}(x) \equiv A^{(i)}(x)\varphi_i^{(i)}(x)/\lambda_i^{(i)}B^{(i)}(x)\varphi_i^{(i)}(x). \quad (78)$$

As we have pointed out earlier, the motivation for replacing $\chi_i^{(i)}(x)$ by $\tilde{\chi}_i^{(i)}(x)$ is that the equation for $\tilde{\chi}_i^{(i)}(x)$ contains no reference to the unknown quantities $\psi_i^{(i)}(x)$ and $\Lambda_i^{(i)}$.

We are now in a position to show the relationship of this work to the Rayleigh quotient for a non-self-adjoint equation. We take the functional $G[\psi_i(x), \psi_i^*(x)]$ to be the Rayleigh quotient as given by Eq. (15). The sum in Eq. (72) then reduces to two terms, and we have

$$F[\varphi_i, \varphi_i^*, \theta_i, \theta_i^*, \lambda_i] = \frac{\int dx\ \varphi_i^*(x)A(x)\varphi_i(x)}{\int dx\ \varphi_i^*(x)B(x)\varphi_i(x)} + \int dx\ \theta_i(x)[A(x)\varphi_i(x) - \lambda_i B(x)\varphi_i(x)] + \int dx\ \varphi_i^*(x)[A^*(x)\varphi_i^*(x) - \lambda_i B^*(x)\varphi_i^*(x)]. \quad (79)$$

We also have

$$\delta G[\psi_i(\xi), \psi_i^*(\xi); x]/\delta\psi_i = \delta G[\psi_i(\xi), \psi_i^*(\xi); x]/\delta\psi_i^* = 0, \quad (80)$$

and hence Eq. (76) gives

$$A^*(x)\chi_i(x) - \Lambda_i B^*(x)\chi_i(x) = 0, \quad (81)$$

$$A(x)\chi_i^*(x) - \Lambda_i B(x)\chi_i^*(x) = 0. \quad (82)$$

These two equations have a particular solution $\chi_i(x) = \chi_i^*(x) = 0$, and thus we can take $\theta_i(x) = \theta_i^*(x) = 0$. Equation (79) then simplifies to

$$F[\varphi_i(x), \varphi_i^*(x)] = \frac{\int dx\ \varphi_i^*(x)A(x)\varphi_i(x)}{\int dx\ \varphi_i^*(x)B(x)\varphi_i(x)}, \quad (83)$$

which is just the Rayleigh quotient we started with. Thus the Rayleigh quotient for non-self-adjoint equations is embedded in the more general variational principle given here.

As a final example, we consider the application of the variational method to the calculation of off-diagonal matrix elements. That is, we consider two eigenfunctions of the same eigenvalue equation,

$$H(x)\psi_i(x) = \Lambda_i\psi_i(x), \tag{84}$$

$$H(x)\psi_k(x) = \Lambda_k\psi_k(x), \tag{85}$$

where $H(x)$ is a real, self-adjoint operator. We consider this particularly simple eigenvalue equation since this is the equation considered by Borowitz and Vassell.[7] A more general equation of the form given by Eq. (1) presents no difficulties. We take the functional of interest to be

$$G[\varphi_i(x), \varphi_k(x)] = \frac{\int dx\, \varphi_k(x)R(x)\varphi_i(x)}{\{[\int dx\, [\varphi_k(x)]^2][\int dx\, [\varphi_i(x)]^2]\}^{\frac{1}{2}}}, \tag{86}$$

where $R(x)$ is an arbitrary, real, self-adjoint operator and $\varphi_i(x)$ and $\varphi_k(x)$ are first-order approximations to $\psi_i(x)$ and $\psi_k(x)$. If the trial functions are assumed to be normalized according to

$$\int dx\, [\varphi_i(x)]^2 = 1, \qquad i = j, k, \tag{87}$$

we find

$$\frac{\delta G[\varphi_i(\xi), \varphi_k(\xi); x]}{\delta\varphi_k} = R(x)\varphi_i(x) - \varphi_k(x)\int d\xi\, \varphi_k(\xi)R(\xi)\varphi_i(\xi), \tag{88}$$

$$\frac{\delta G[\varphi_i(\xi), \varphi_k(\xi); x]}{\delta\varphi_k} = R(x)\varphi_k(x) - \varphi_i(x)\int d\xi\, \varphi_k(\xi)R(\xi)\varphi_i(\xi). \tag{89}$$

Thus Eqs. (72) and (77) in this special case are written

$$F[\varphi_i(x), \varphi_k(x), \theta_i(x), \theta_k(x), \lambda_i, \lambda_k] = \int dx\, \varphi_k(x)R(x)\varphi_i(x) + \int dx\, \theta_i(x)[H(x)\varphi_i(x) - \lambda_i\varphi_i(x)] + \int dx\, \theta_k(x)[H(x)\varphi_k(x) - \lambda_k\varphi_k(x)], \tag{90}$$

$$\varphi_i(x)H(x)\tilde{\chi}_i(x) - \tilde{\chi}_i(x)H(x)\varphi_i(x) = \varphi_i(x)R(x)\varphi_k(x) - \varphi_i^2(x)\int d\xi\, \varphi_k(\xi)R(\xi)\varphi_i(\xi), \tag{91}$$

$$\varphi_k(x)H(x)\tilde{\chi}_k(x) - \tilde{\chi}_k(x)H(x)\varphi_k(x) = \varphi_k(x)R(x)\varphi_i(x) - \varphi_k^2(x)\int d\xi\, \varphi_k(\xi)R(\xi)\varphi_i(\xi). \tag{92}$$

To make clear the correspondence of Eqs. (90)–(92) to the variational principle of Borowitz and Vassell, we define the quantities $j(x)$, $k(x)$, $J(x)$, $K(x)$, $J'(x)$, $K'(x)$, $\langle E_i\rangle$, and $\langle E_k\rangle$ by the equations

$$\varphi_i(x) \equiv j(x), \tag{93}$$

$$\varphi_k(x) \equiv k(x), \tag{94}$$

$$\theta_i(x) \equiv j(x)J(x), \tag{95}$$

$$\theta_k(x) \equiv -k(x)K(x), \tag{96}$$

$$\tilde{\chi}_i(x) \equiv j(x)J'(x), \tag{97}$$

$$\tilde{\chi}_k(x) \equiv -k(x)K'(x), \tag{98}$$

$$\lambda_i \equiv \langle E_i\rangle, \tag{99}$$

$$\lambda_k \equiv \langle E_k\rangle. \tag{100}$$

The primes in Eqs. (97) and (98) are used to distinguish these quantities from the corresponding unprimed quantities in Eqs. (95) and (96) and do not imply differentiation. We further make use of the commutator symbol [,] for two operators $A(x)$ and $B(x)$,

$$[A, B] \equiv A(x)B(x) - B(x)A(x), \tag{101}$$

and Dirac notation, e.g.,

$$A(x)j(x) \equiv A\,|j\rangle, \tag{102}$$

$$k(x)A(x) \equiv \langle k|\,A, \tag{103}$$

$$\int dx\, j(x)A(x)k(x) \equiv \langle j|\,A\,|k\rangle. \tag{104}$$

With these definitions and notation, Eqs. (90)–(92) can be written

$$F[j, k, J, K, \langle E_i\rangle, \langle E_k\rangle] = \langle k|\,R\,|j\rangle - \langle j|\,J\langle E_i\rangle - HJ\,|j\rangle - \langle k|\,KH - \langle E_k\rangle K\,|k\rangle, \tag{105}$$

$$\langle j|\,[J', H] = \langle k|\,Q, \tag{106}$$

$$[K', H]\,|k\rangle = Q\,|j\rangle, \tag{107}$$

where we have defined the operator Q as

$$Q \equiv R - |k\rangle\langle k|\,R\,|j\rangle\langle j|. \tag{108}$$

Equations (105)–(108) are just Eqs. (2.5), (2.6), (2.7), and (2.22) of Borowitz and Vassell. Hence we see that the formalism given in this paper con-

tains the variational principle of Borowitz and Vassell as a special case.

Two final points should be made. In the first place, J and K in Eq. (105) are meant as first-order approximations to J' and K' as defined by Eqs. (106) and (107). In the paper of Borowitz and Vassell, only one set of functions, J and K, is introduced, implying that an exact solution of Eqs. (106) and (107) is required for use in the functional, Eq. (105). We see from the present work, however, that this is not the case. Secondly, Borowitz and Vassell imply that $\langle E_i \rangle$ and $\langle E_k \rangle$ in Eq. (105) must either be the exact eigenvalues or differ from the exact results by second-order terms (e.g., as calculated from the Rayleigh quotient). This is the case if one uses any solution, or a first-order approximation to any solution of Eqs. (106) and (107) as the trial functions. However, as we have shown, if one chooses a particular solution, or a first-order approximation to this particular solution, for J' and K', all that is required of $\langle E_i \rangle$ and $\langle E_k \rangle$ is that they be first-order approximations to the exact eigenvalues. These same points have been discussed by Borowitz and Gerjuoy.[8]

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