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Construction of Vanishing Cycles for Integrals over Hyperspheres*

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The homological methods of Fotiadi *et al.* are applied to the study of the analytic properties of an integral over a l-sphere Γ of a closed meromorphic l-form on the complex quadric of which Γ is the real section. Vanishing cycles are explicitly constructed at points of a certain standard type, and the relevant Kronecker indices are evaluated. The Picard–Lefschetz theorem and the decomposition theorem are then applied to obtain linear relations between the discontinuities round various singularities. The results have a direct physical interpretation in the cases $l = 4$ and $l = 2$ in terms of the Riemann sheet structure of single-loop Feynman diagrams with four, five, or six vertices. They give linear relations between the various discontinuity functions, which generalize the results obtained by Fotiadi and Pham for the two-particle discontinuity of the five-point loop and for the complete Feynman amplitude of the four-point loop.

1. INTRODUCTION

THE methods of homology theory have been applied by Fotiadi and Pham[1,2] to the study of the analytic properties of various Feynman and unitarity integrals. In all the simplest cases, the first step is to convert the integral into an integral over a hypersphere. Thus, two-particle unitarity integrals are expressed as integrals over 2-spheres[1] and Feynman integrals of single-loop diagrams with four or more vertices as integrals over 4-spheres.[2] The Picard–Lefschetz theorem and the decomposition theorem of Fotiadi *et al.*[3] are used to derive relations between the discontinuities round paths encircling the various Landau surfaces. To obtain the actual form of these relations in a particular case, it is necessary to know certain Kronecker indices. In the two cases they considered, Fotiadi and Pham[1,2] give values for the Kronecker indices in question, but they omit the argument leading to these values. We shall consider the general case of an integral over an l-sphere, construct a set of vanishing cycles at a point of a certain standard type to be specified, and evaluate the relevant Kronecker indices.

The integral to be studied is of the type

$$J(P) = \int_\Gamma \frac{f\omega}{\prod_{j=1}^{m} (\mathbf{p}_j \cdot \mathbf{z} - 1)^{a_j}}, \qquad (1.1)$$

where the integrand is a closed meromorphic l-form on the complex quadric

$$\Sigma = \{(z_0, z_1, \cdots, z_l) \in \mathbf{C}^{l+1}: z_0^2 + z_1^2 + \cdots + z_l^2 = 1\},$$

and the cycle of integration is the l-sphere

$$\Gamma = \{(x_0, x_1, \cdots, x_l) \in \mathbf{R}^{l+1}: x_0^2 + x_1^2 + \cdots + x_l^2 = 1\}$$

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[1] D. Fotiadi and F. Pham, "Landau–Cutkosky Rules for Unitarity Integrals" (1963) (Unpublished).
[2] D. Fotiadi and F. Pham, "Analytic Study of some Feynman Graphs by Homological Method," Ecole Polytechnique, Paris (1963) (Unpublished).
[3] D. Fotiadi, M. Froissart, J. Lascoux, and F. Pham, Topology 4, 159 (1965).

oriented as the boundary of the canonically oriented closed $(l+1)$–ball

$$\{(x_0, x_1, \cdots, x_l) \in \mathbf{R}^{l+1}: x_0^2 + x_1^2 + \cdots + x_l^2 \leq 1\}.$$

The positive integers l, m, and q_j satisfy

$$q = \sum_{j=1}^{m} q_j \geq l.$$

f is a polynomial in $z_0, z_1, \cdots, z_l$ of degree $q - l$ at most. For technical reasons connected with the existence of the standard points at which we propose to construct vanishing cycles, we shall also have to impose the restriction that

$$m \leq l + 2.$$

ω is the closed holomorphic l-form

$$\omega = \sum_{i=0}^{l} (-1)^i z_i \, dz_0 \wedge \cdots \wedge \widehat{dz_i} \wedge \cdots \wedge dz_l|_{\mathbf{z}},$$

where a hat over a symbol indicates that it is to be omitted from the product in which it occurs. The symbol $\mathbf{a}\cdot\mathbf{b}$ for a pair of complex n–vectors $\mathbf{a} = (a_1, a_2, \cdots, a_n)$ and $\mathbf{b} = (b_1, b_2, \cdots, b_n)$ stands for the scalar product

$$\mathbf{a}\cdot\mathbf{b} = \sum_{i=1}^{n} a_i b_i.$$

The symbol P stands for the m complex $(l+1)$–vectors $\mathbf{p}_j$, and we shall study the analytic properties of $J(P)$ as a function of $P \in \mathbf{C}^{m(l+1)}$. In some physical applications, the components of the $\mathbf{p}_j$ are not all independent, they rather depend holomorphically on some parameter t varying in a complex analytic manifold T of lower dimension. Then J should be regarded as a function of t rather than of P. It usually happens, however, that there is still sufficient freedom in the $\mathbf{p}_j$ (at least if we allow analytic continuation in particle masses) to enable us to vary them along paths of the types to be described later. We shall therefore regard the components of the $\mathbf{p}_j$ as independent complex variables and consider J as an analytic function of P in $\mathbf{C}^{m(l+1)}$.

To bring the integral (1.1) into the standard form discussed by Fotiadi *et al.*,[3] it is necessary to compactify the ambient manifold Σ of the cycle of integration. This is most simply achieved by changing to homogeneous coordinates. Putting

$$z_i = \zeta_i/\zeta_{l+1} \qquad (i = 0, 1, \cdots, l),$$

and making the change of variable in the integral (1.1), we obtain

$$J(P) = \int_{\Gamma} \frac{\bar{f}\bar{\omega}}{\prod_{j=1}^{m} (\bar{\mathbf{p}}_j\cdot\zeta)^{q_j}}, \tag{1.2}$$

where $\bar{f} = (\zeta_{l+1})^{q-l} f(\zeta_0/\zeta_{l+1}, \cdots, \zeta_l/\zeta_{l+1})$ is a homogeneous polynomial of degree $q - l$ in $\zeta_0, \zeta_1, \cdots, \zeta_{l+1}$, $\bar{\omega}$ is the differential l–form

$$\bar{\omega} = (\zeta_{l+1})^{-1} \sum_{i=0}^{l} (-1)^i \zeta_i \, d\zeta_0 \wedge \cdots \wedge \widehat{d\zeta_i} \wedge \cdots \wedge d\zeta_l|_{\bar{\mathbf{z}}},$$

and $\bar{\mathbf{p}}_j$ is the complex $(l+2)$–vector $(\mathbf{p}_j, -1)$. The new ambient manifold is the complex projective quadric

$$\bar{\Sigma} = [(\zeta_0, \zeta_1, \cdots, \zeta_{l+1}) \in P^{l+1}(\mathbf{C}): \zeta_0^2 + \cdots + \zeta_l^2 = (\zeta_{l+1})^2]$$

which is compact. $\bar{\Gamma}$ is the homeomorphic image of Γ under the map ϖ: $\mathbf{C}^{l+1} \to P^{l+1}(\mathbf{C})$ defined by $\varpi(z_0, \cdots, z_l) = (z_0, \cdots, z_l, 1)$, which maps $\mathbf{C}^{l+1}$ homeomorphically onto $P^{l+1}(\mathbf{C}) - P^l_\infty(\mathbf{C})$, where $P^l_\infty(\mathbf{C})$ is the hyperplane, $\zeta_{l+1} = 0$, of $P^{l+1}(\mathbf{C})$. For each integer j satisfying $0 \leq j \leq l$, it is easy to show by eliminating $d\zeta_j$ that

$$\bar{\omega} = (-1)^{j+l}(\zeta_j)^{-1}\Big[\sum_{i<j} (-1)^i \zeta_i \, d\zeta_0 \wedge \cdots \wedge \widehat{d\zeta_i} \wedge \cdots \wedge \widehat{d\zeta_j} \wedge \cdots \wedge d\zeta_{l+1} + \sum_{i>j} (-1)^{i-1} \zeta_i \, d\zeta_0 \wedge \cdots \wedge \widehat{d\zeta_j} \wedge \cdots \wedge \widehat{d\zeta_i} \wedge \cdots \wedge d\zeta_{l+1}\Big]|_{\bar{\mathbf{z}}}.$$

Since $\zeta = \mathbf{0}$ does not define a point of $P^{l+1}(\mathbf{C})$, it follows that $\bar{\omega}$ is a regular form on $\bar{\Sigma}$.

We write P_j for the hyperplane $\mathbf{p}_j\cdot\mathbf{z} = 1$ in $\mathbf{C}^{l+1}$, $\bar{P}_j$ for the corresponding hyperplane $\bar{\mathbf{p}}_j\cdot\zeta = 0$ in $P^{l+1}(\mathbf{C})$, $\Sigma_j = \Sigma \cap P_j$ and $\bar{\Sigma}_j = \bar{\Sigma} \cap \bar{P}_j$. The integrand of (1.2) is holomorphic except on the $(l-1)$-dimensional complex analytic submanifolds $\bar{\Sigma}_j$ of $\bar{\Sigma}$. Let Φ be the domain of $\mathbf{C}^{m(l+1)}$ defined by the inequalities

$$|\mathrm{Re}\ \mathbf{p}_j| < 1 \qquad (j = 1, 2, \cdots, m).$$

The standard points (to be defined at the beginning of Sec. 3) all belong to Φ. For $P \in \Phi$, the cycle $\bar{\Gamma}$ of integration does not intersect any of the $\bar{\Sigma}_j$.

Hence, the integral (1.2) is well defined and holomorphic in Φ. It follows from the isotopy theorem of Fotiadi *et al.*[3] that (1.2) may be analytically continued away from Φ along any path on which the $\bar{\Sigma}_j$ remain in general position, the cycle $\bar{\Gamma}$ of integration being deformed by the ambient isotopy associated with the path. This analytic continuation can only be blocked when a point is reached at which the $\bar{\Sigma}_j$ are no longer in general position. Because of the particularly simple form of (1.2), this can only happen when there is a simple pinch involving the $\bar{\Sigma}_j$ for $j \in \beta$, where β is some subset of $\{1, \cdots, m\}$ such that the number $|\beta|$ of its elements satisfies $1 \leq |\beta| \leq l + 1$. The set of all such β will be called B. The condition for a simple pinch in the system β is that there exists a point $\bar{\mathbf{q}} = (\mathbf{q}, q_{l+1})$ of $P^{l+1}(\mathbf{C})$ and complex numbers λ_j $(j \in \beta)$ such that

$$\left.\begin{aligned} &\mathbf{q}^2 = (q_{l+1})^2, \qquad \mathbf{p}_j \cdot \mathbf{q} = q_{l+1} \qquad (j \in \beta), \\ &\mathbf{q} = \sum_{j\in\beta} \lambda_j \mathbf{p}_j, \qquad \sum_{j\in\beta} \lambda_j = q_{l+1}. \end{aligned}\right\} \tag{1.3}$$

This is possible if (and only if) P lies on the Landau surface L_β whose equation is

$$L_\beta(P) \equiv \det (\mathbf{p}_i \cdot \mathbf{p}_j - 1)_{i,j\in\beta} = 0.$$

Thus, the singularities of $J(P)$ lie on the Landau surfaces L_β, which are complex analytic submanifolds of $\mathbf{C}^{m(l+1)}$ of co-dimension 1, and $J(P)$ may be continued along any path in

$$\mathbf{C}^{m(l+1)} - \bigcup_{\beta\in B} L_\beta.$$

$J(P)$ is not a single-valued function of P, because some of the L_β correspond to branch-point singularities. Continuation of $J(P)$ round a closed loop based on a point P_0 of Φ and encircling some of the L_β will produce, instead of the original $J(P_0)$ integrated over $\bar{\Gamma}$, an integral of the same form over a cycle of integration obtained from $\bar{\Gamma}$ by applying the ambient isotopy associated with the loop. Since the integrand is a closed form, the integral will depend only on the homology class of the cycle of integration in the compact homology group $H_l^c(\bar{\Sigma} - \bigcup_{j=1}^m \bar{\Sigma}_j)$. Thus, $J(P)$ depends both on P and on the homology class of its cycle of integration. The latter tells us which "Riemann sheet" we are on. We investigate the Riemann sheet structure by studying the effect on $J(P)$ of successive continuations round a sequence of closed loops based on a standard point, each loop encircling one of the L_β.

In Sec. 2, we explain what we mean by vanishing cycles and why they are of importance in this problem. The geometrical construction of the cycles is carried out in Sec. 3, where it is shown that they are indeed vanishing cycles. The orientation of the cycles is specified in Sec. 4, where the relevant Kronecker indices are evaluated. Finally, in Sec. 5, the decomposition theorem is used to obtain linear relations between the discontinuities of $J(P)$ around its various Landau surfaces L_β.

The results obtained have a direct physical interpretation in the case $l = 4$. The Feynman integral corresponding to a single-loop diagram with m vertices (where $m \geq 4$) may be cast[2] into the form (1.2) with $l = 4$, $q_j = 1$, and $\bar{f} = (\zeta_4 + \zeta_5)^{m-4}$. Each factor $\bar{\mathbf{p}}_j \cdot \zeta$ in the denominator of the integrand corresponds to an internal line j of the diagram, and L_β is the Landau surface obtained by putting the lines j in β on the mass shell and contracting out all the other internal lines. Thus, our results give information about the Riemann sheet structure of single-loop diagrams with four, five, or six vertices. Similarly, in the case $l = 2$, we obtain information about the two-particle discontinuities (as evaluated by the Cutkosky prescription) of Feynman diagrams of these three types.[1]

2. THE NATURE OF THE PROBLEM

We outline the program to be carried through in Secs. 3, 4, and 5.

In Secs. 3 and 4, we construct at each standard point a set of relative cycles e_β, one for each β in B. e_β is a compact l-chain of Σ with boundary in ${}_{(\beta)}\Sigma$, where

$${}_{(\beta)}\Sigma = \bigcup_{j\in\beta} \Sigma_j, \qquad {}^{(\beta)}\Sigma = \bigcap_{j\in\beta} \Sigma_j,$$

and a similar notation is employed for the $\bar{\Sigma}_j$. The homeomorphic image of the above chain under ϖ defines a compact l-chain of $\bar{\Sigma}$ with boundary in ${}_{(\beta)}\bar{\Sigma}$. By abuse of language, we shall denote this chain and its relative homology class in $H_l^c(\bar{\Sigma}, {}_{(\beta)}\bar{\Sigma})$ by the same symbol e_β. If $\beta = \{i_1 i_2 \cdots i_r\}$, we can write

$$e_\beta = e_{i_1 i_2 \cdots i_r},$$

the order of the indices being immaterial. If $1 \leq s \leq r$, we define

$$e^{i_1 \cdots i_s}{}_{i_{s+1} \cdots i_r} = \partial_{i_s} \cdots \partial_{i_2} \partial_{i_1} e_{i_1 \cdots i_r} \in H_{l-s}^c\Big(\bigcap_{k=1}^{s} \bar{\Sigma}_{i_k}, \bigcup_{k=s+1}^{r} \bar{\Sigma}_{i_k}\Big),$$

where the ∂_i are boundary homomorphisms. Geometrically, the operator ∂_i applied to a relative cycle gives the part of its boundary which lies in

$\bar{\Sigma}_i$. As the different boundary homomorphisms anticommute, it follows that $e^{i_1 \cdots i_s}{}_{i_{s+1} \cdots i_r}$ is antisymmetric in its superscripts though symmetric in its subscripts. The cycle $e^{i_1 \cdots i_r}$ is an $(l - r)$-sphere for $r \leq l$, and is zero for $r = l + 1$. It will be shown that $e^{i_1 \cdots i_r}$ does not intersect any $\bar{\Sigma}_i$ with $j \in \bar{\beta}$, where $\bar{\beta}$ is the complement of β in $\{1, \cdots, m\}$, so that it defines an element of $H^c_{l-r}({}^{(\beta)}\bar{\Sigma} - {}_{(\bar{\beta})}\bar{\Sigma})$, which will again be denoted by $e^{i_1 \cdots i_r}$, or, when a definite order of the elements of β is understood, simply by e^β.

In Sec. 3, we construct, for a given standard point P_0 and a given β in B a path λ_β: $[0, 1] \to \mathbf{C}^{m(l+1)}$ such that

$$\lambda_\beta(0) = P_0, \qquad \lambda_\beta(1) = P_\beta,$$

$$\lambda_\beta(t) \in \Phi \cap \{\mathbf{C}^{m(l+1)} - \bigcup_{\gamma \in B} L_\gamma\}, \quad \text{for} \quad 0 \leq t < 1,$$

where

$$P_\beta \in L_\beta$$

but

$$P_\beta \notin L_\gamma, \quad \text{for} \quad \gamma \in B, \qquad \gamma \neq \beta.$$

At P_β there will be a simple pinch in the system β such that the point $\bar{\mathfrak{q}}$ satisfying (1.3) lies on the original undeformed cycle of integration $\bar{\Gamma}$. The definition of e_β will be extended from P_0 to the whole of λ_β in such a way that e_β depends continuously on t and shrinks to a point (in fact to the point $\bar{\mathfrak{q}}$ mentioned above) as $t \to 1$. The cycle e^β, and the various relative cycles also obtained from e_β by repeated application of boundary homomorphisms, clearly also have this property. It is for this reason that they are called vanishing (relative) cycles.

Now, it follows from the proof of the Picard–Lefschetz theorem[3] that there exists an open ball W in $\bar{\Sigma}$ centered on $\bar{\mathfrak{q}}$ and a neighborhood V of P_β in $\mathbf{C}^{m(l+1)}$ such that, for $P \in V$, $W \cap \bar{\Sigma}_j(P)$ is empty for $j \notin \beta$, while the $W \cap \bar{\Sigma}_i(P)$ for $j \in \beta$ are in general positioned in W except when $P \in L_\beta$. For t sufficiently close to 1, the point $\lambda_\beta(t)$ lies in V, and the corresponding e_β is contained in W. Let Q_β be any such point, and let α_β be a closed loop based on P_0 made up of the part $\bar{\lambda}_\beta$ of λ_β from P_0 to Q_β followed first by a small circuit γ_β about P_β in a positive sense (that which makes arg L_β increase by 2π) and then by a return from Q_β to P_0 along $\bar{\lambda}_\beta$ described in reverse. The proof of the Picard–Lefschetz theorem shows that, for $|\beta| \leq l$, the compact relative homology group $H^c_l(W, {}_{(\beta)}\bar{\Sigma} \cap W)$ at Q_β is an infinite cyclic group (written additively). As e_β is contained in W, it defines an element of this homology group, which must in fact generate the whole group. Similarly, the reduced homology group $\tilde{H}^c_{l-|\beta|}({}^{(\beta)}\bar{\Sigma} \cap W)$ is an infinite cyclic group and is generated by the iterated boundary e^β of e_β. According to the Picard–Lefschetz theorem, the ambient isotopy associated with the small loop γ_β induces an automorphism of $H^c_p(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i)$ at Q_β which is the identity except in the case $p = l \geq |\beta|$, when an element h of $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i)$ undergoes the change

$$h \to h + n i_* \, \delta^{|\beta|} e^\beta, \tag{2.1}$$

where

$$n = (-1)^{\frac{1}{2}(l-|\beta|+1)(l-|\beta|+2)} \mathrm{KI}\,[h, e_\beta], \tag{2.2}$$

in which KI means Kronecker index (to be defined in Sec. 4). $\delta^{|\beta|}$ is the iterated coboundary operator as defined by Fotiadi *et al.*[3] This definition differs in sign from that of Leray.[4] Since different coboundary operators anticommute, their order is important. If $\beta = \{i_1 \cdots i_r\}$, the symbol $\delta^{|\beta|} e^\beta$ stands for

$$\delta_{i_1} \cdots \delta_{i_r} e^{i_1 \cdots i_r} = \delta_{i_1} \cdots \delta_{i_r} \partial_{i_r} \cdots \partial_{i_1} e_\beta,$$

which is independent of the order of the symbols $i_1 \cdots i_r$. $\delta^{|\beta|} e^\beta$ is an element of $H^c_l(W - {}_{(\beta)}\bar{\Sigma} \cap W)$. i_* is the homology homomorphism induced by the inclusion map

$$i : W - {}_{(\beta)}\bar{\Sigma} \cap W \to \bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i.$$

The formula (2.1) remains valid when $|\beta| = l + 1$, as e^β then vanishes. Now, the ambient isotopy associated with the path $\bar{\lambda}_\beta$ sends e_β and e^β at P_0 to the corresponding homology classes at Q_β and it preserves Kronecker indices. It follows that the ambient isotopy associated with the loop α_β induces an automorphism ψ_β of $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i)$ at P_0, given by

$$h \to \psi_\beta(h) = h + n \, \delta^{|\beta|} e^\beta, \quad h \in H^c_l\Big(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i\Big), \tag{2.3}$$

where n is given by an expression having the same appearance as (2.2), but involving homology classes at P_0 instead of at Q_β. In (2.3), e^β is to be regarded as an element of $H^c_{l-|\beta|}({}^{(\beta)}\bar{\Sigma} - {}_{(\bar{\beta})}\bar{\Sigma})$, so that $\delta^{|\beta|} e^\beta$ is indeed an element of $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i)$.

Now, as we saw towards the end of the introduction, the value of $J(P_0)$ on a particular Riemann sheet depends linearly on the homology class of the cycle of integration corresponding to that sheet. Hence, in order to ascertain what happens to $J(P)$ when it is continued around a succession of loops

[4] J. Leray, Bull. Soc. Math. France 87, 81 (1959).

α_β, it is sufficient to find the images of the homology class of the original cycle of integration Γ under successive applications of the automorphisms ψ_β. We see from (2.2) and (2.3) that, in order to do this, we must know the Kronecker indices of Γ and the $\delta^{|\beta|}e^\beta$ with the e_β. These Kronecker indices are found in Sec. 4. In Sec. 5, we use the decomposition theorem to obtain a basis for the group $H_l^i(\bar{\Sigma} - \bigcup_{j=1}^m \bar{\Sigma}_j)$, and find the matrix representations of the ψ_β with respect to this basis. Linear relations between some of the $\delta^{|\beta|}e^\beta$ and (when l is odd) Γ are also obtained. These can immediately be translated into linear relations between the discontinuity functions

$$A_\beta(P) = -n \int_{\delta^{|\beta|}e^\beta} \frac{\bar{f}\bar{\omega}}{\prod_{j=1}^m (\bar{\mathbf{p}}_j \cdot \zeta)^{\alpha_j}}. \tag{2.4}$$

The minus sign has been inserted in (2.4) to agree with the convention usual among physicists that the discontinuity is the original value minus the analytic continuation around L_β in a positive sense.

3. CONSTRUCTION OF VANISHING CYCLES

By a standard point we mean a point P of $\mathbf{C}^{m(l+1)}$ at which the $\mathbf{p}_j$ are all real, their lengths $|\mathbf{p}_j|$ are all less than unity, and the following conditions are satisfied for each β in B:

(i) The $\mathbf{p}_j$ for $j \in \beta$ are linearly independent, so that their Gram determinant $\Delta^{(\beta)}$ is positive.

(ii) $\Delta_j^{(\beta)} > 0$ for each j in β, where $\Delta_j^{(\beta)}$ is the determinant obtained from $\Delta^{(\beta)}$ by replacing the column corresponding to $\mathbf{p}_j$ by a column filled with 1's.

The condition $m \leq l + 2$ ensures that such points exist. For $m = l + 2$ one could take $\mathbf{p}_1, \cdots, \mathbf{p}_m$ to be the position vectors of the vertices of a regular $(l + 1)$-simplex centered at the origin. We define

$$\pi_\beta = \{\Delta^{(\beta)}\}^{-1} \sum_{j\in\beta} \Delta_j^{(\beta)} \mathbf{p}_j \qquad (\beta \in B). \tag{3.1}$$

Then

$$\mathbf{p}_j \cdot \pi_\beta = 1, \quad \text{for} \quad j \in \beta. \tag{3.2}$$

This implies, since $|\mathbf{p}_j| < 1$, that

$$\pi_\beta^2 = \{\Delta^{(\beta)}\}^{-1} \sum_{j\in\beta} \Delta_j^{(\beta)} > 1. \tag{3.3}$$

Hence,

$$L_\beta(P) = \det(\mathbf{p}_i \cdot \mathbf{p}_j - 1)_{i,j\in\beta} = \Delta^{(\beta)} - \sum_{j\in\beta} \Delta_j^{(\beta)} < 0.$$

Thus, a standard point cannot lie on a Landau surface of $J(P)$. The vector

$$\mathbf{p}_\beta = (\pi_\beta^2)^{-1}\pi_\beta = \{\sum_{j\in\beta} \Delta_j^{(\beta)}\}^{-1} \sum_{j\in\beta} \Delta_j^{(\beta)} \mathbf{p}_j \tag{3.4}$$

is the perpendicular from the origin onto the $(|\beta|-1)$-plane through the end-points of the $\mathbf{p}_j$ with $j \in \beta$. Condition (ii) expresses the requirement that the foot of this perpendicular should lie inside the $(|\beta| - 1)$-simplex spanned by the $\mathbf{p}_j$ with $j \in \beta$. When β and γ are elements of B such that γ is a proper subset of β, we have the identities

$$\mathbf{p}_\gamma \cdot \pi_\beta = 1, \qquad \pi_\beta \cdot \pi_\gamma = \pi_\gamma^2, \qquad \mathbf{p}_\beta \cdot \mathbf{p}_\gamma = \mathbf{p}_\beta^2, \tag{3.5}$$

and the inequalities

$$\pi_\beta^2 > \pi_\gamma^2, \qquad \mathbf{p}_\beta^2 < \mathbf{p}_\gamma^2 \tag{3.6}$$

which follow simply from the definitions and conditions (i) and (ii).

Let P be a given standard point and β a given element of B. We define the relative cycle e_β to be the sum of two chains $e_\beta^{(1)}$ and $e_\beta^{(2)}$. These chains are specified by giving their supports and then orienting them. The supports are subsets of $\Sigma \subset \mathbf{C}^{l+1}$ and, in giving them, we write $\mathbf{z}$ for a general complex $(l + 1)$-vector and $\mathbf{x}$ and $\mathbf{y}$ for its real and imaginary parts. The support $|e_\beta^{(1)}|$ of $e_\beta^{(1)}$ is the set of all $\mathbf{z}$ in $\mathbf{C}^{l+1}$ such that

$$\begin{aligned} &\mathbf{x} = \lambda\, |\pi_\beta|^{-1} \pi_\beta, \qquad \pi_\beta \cdot \mathbf{y} = 0, \\ &\mathbf{y}^2 = \lambda^2 - 1, \qquad 1 \leq \lambda \leq |\pi_\beta|. \end{aligned} \tag{3.7}$$

The chain $e_\beta^{(2)}$ is defined to be zero when $|\beta| = 1$. For $|\beta| > 1$, the support $|e_\beta^{(2)}|$ of $e_\beta^{(2)}$ is the set of all $\mathbf{z}$ in $\mathbf{C}^{l+1}$ such that *either*

$$\mathbf{x} = \pi_\beta, \qquad \pi_\beta \cdot \mathbf{y} = 0, \qquad \mathbf{y}^2 = \pi_\beta^2 - 1$$

or

$$\begin{aligned} &\mathbf{x} \cdot (\pi_\beta - \mathbf{x}) = 0, \qquad \mathbf{x} \neq \pi_\beta, \\ &\mathbf{p}_j \cdot \mathbf{x} \geq 1 \text{ for some } j \in \beta, \\ &\mathbf{y} = (\mathbf{x}^2 - 1)^{\frac{1}{2}}\, |\mathbf{x} - \pi_\beta|^{-1} (\mathbf{x} - \pi_\beta). \end{aligned} \tag{3.8}$$

The orientations of the chains $e_\beta^{(1)}$ and $e_\beta^{(2)}$ are given in Sec. 4. There it is shown that, for $|\beta| > 1$, the boundary $\partial e_\beta^{(1)}$ of $e_\beta^{(1)}$ occurs as a term in $\partial e_\beta^{(2)}$, but with opposite orientation. Hence, $\partial e_\beta^{(1)}$ does not appear in the boundary ∂e_β of e_β, and the latter is of the form $\bigcup_{j\in\beta} \partial_j e_\beta$, where $|\partial_j e_\beta|$ is the set of all $\mathbf{z}$ in $\mathbf{C}^{l+1}$ such that

$$\begin{aligned} &\mathbf{x} \cdot (\pi_\beta - \mathbf{x}) = 0, \qquad \mathbf{x} \neq \pi_\beta, \qquad \mathbf{p}_j \cdot \mathbf{x} = 1, \\ &\mathbf{p}_i \cdot \mathbf{x} \leq 1 \quad \text{for} \quad i \in \beta - \{j\}, \\ &\mathbf{y} = (\mathbf{x}^2 - 1)^{\frac{1}{2}}\, |\mathbf{x} - \pi_\beta|^{-1} (\mathbf{x} - \pi_\beta), \end{aligned} \tag{3.9}$$

when $|\beta| > 2$ and the closure of the above set when $|\beta| = 2$. Thus, the boundary of e_β lies in ${}_{(\beta)}\Sigma$ for

$|\beta| > 1$ and clearly also for $|\beta| = 1$. Hence, e_β is indeed a relative cycle of the type specified in Sec. 2. If $\beta = \{i_1, i_2, \cdots, i_r\}$ and $0 < s < r$, we note, as a generalization of (3.9), that $|e^{i_1 \cdots i_s}_{i_{s+1} \cdots i_r}|$ is the closure of the set of all $\mathbf{z}$ in $\mathbf{C}^{l+1}$ such that

$$\mathbf{x}\cdot(\pi_\beta - \mathbf{x}) = 0, \quad \mathbf{x} \neq \pi_\beta, \quad \mathbf{p}_j\cdot\mathbf{x} = 1$$

for

$$j \in \{i_1 \cdots i_s\}, \quad \mathbf{p}_j\cdot\mathbf{x} \leq 1 \quad \text{for} \quad j \in \{i_{s+1} \cdots i_r\},$$
$$\mathbf{y} = (\mathbf{x}^2 - 1)^{\frac{1}{2}} |\mathbf{x} - \pi_\beta|^{-1} (\mathbf{x} - \pi_\beta). \tag{3.10}$$

For the cycle e^β, we have

$$|e^\beta| = \{\mathbf{z} \in \mathbf{C}^{l+1}:$$
$$\mathbf{x} = \pi_\beta, \mathbf{p}_j\cdot\mathbf{y} = 0 \ \forall\ j \in \beta, \mathbf{y}^2 = \pi_\beta^2 - 1\}. \tag{3.11}$$

This is a $(l - |\beta|)$-sphere if $|\beta| \leq l$. For $|\beta| = l + 1$, $|e^\beta|$ is empty and e^β is zero. To demonstrate that, when $|\beta| \leq l$, $|e^\beta|$ does not intersect any Σ_j with $j \notin \beta$, it suffices to observe that, if $j \notin \beta$,

$$\mathbf{p}_j\cdot\pi_\beta - 1 = \{\Delta^{(\beta)}\}^{-1} \sum_{i\in\beta} \Delta_i^{(\beta)} \mathbf{p}_i\cdot\mathbf{p}_j - 1$$
$$= -\{\Delta^{(\beta)}\}^{-1} \Delta_j^{(\beta j)} < 0, \tag{3.12}$$

where βj is a shorthand for $\beta \cup \{j\}$.

Our next task is to construct a path λ_β for a given standard point P_0 and a given β in B. We define λ_β to be $\lambda_\beta^{(1)}$ followed by $\lambda_\beta^{(2)}$, where $\lambda_\beta^{(1)}$ is a path of standard points starting at P_0 and ending at a point $P'_\beta(\mathbf{p}_j = \mathbf{p}'_j)$, where $(\mathbf{p}'_\beta)^2$ is close to unity (so that the vectors $\mathbf{p}'_j$ for $j \in \beta$ are almost parallel and of length just less than unity) but the $(\mathbf{p}'_\gamma)^2$ for $\gamma \not\subset \beta$ are not close to unity. Thus P'_β is close to the L_γ with $\gamma \subset \beta$ but not to those with $\gamma \not\subset \beta$. For $0 \leq t \leq 1$, $\lambda_\beta^{(2)}(t)$ is defined to be the point given by

$$\mathbf{p}_j = (1 - t)\mathbf{p}'_j + t\mathbf{q} + i\lambda t(\mathbf{p}'_\beta - \mathbf{p}'_j)$$
$$\text{for} \quad j \in \beta, \tag{3.13}$$
$$\mathbf{p}_j = \mathbf{p}'_j \quad \text{for} \quad j \notin \beta,$$

where

$$\mathbf{q} = |\mathbf{p}'_\beta|^{-1} \mathbf{p}'_\beta \tag{3.14}$$

and λ is a small positive number. The corresponding value of $\mathbf{p}_\gamma$ for $\gamma \subset \beta$ is given by

$$\mathbf{p}_\gamma = (1 - t)\mathbf{p}'_\gamma + t\mathbf{q} + i\lambda t(\mathbf{p}'_\beta - \mathbf{p}'_\gamma) \tag{3.15}$$

as can easily be verified. In particular,

$$\mathbf{p}_\beta = \{t + (1 - t)\eta\}\mathbf{q}, \tag{3.16}$$

where

$$\eta = |\mathbf{p}'_\beta|. \tag{3.17}$$

For $0 \leq t < 1$, it is clear that $\lambda_\beta^{(2)}(t) \in \Phi$. Moreover, $\lambda_\beta^{(2)}(t) \notin L_\gamma$ for $\gamma \subset \beta$, as $\mathbf{p}_\gamma^2 \neq 1$ (see Eq. 3.3). This is true because $\operatorname{Im} \mathbf{p}_\gamma^2 < 0$ for $0 < t < 1$ when γ is a proper subset of β and $\mathbf{p}_\beta^2 < 1$ for $0 \leq t < 1$. At $P_\beta = \lambda_\beta^{(2)}(1)$ we have

$$\mathbf{p}_j = \mathbf{q} + i\lambda(\mathbf{p}'_\beta - \mathbf{p}'_j), \quad \text{for} \quad j \in \beta.$$

The conditions (1.3) are satisfied at P_β with

$$\bar{\mathbf{q}} = (\mathbf{q}, 1) \in \bar{\Gamma}, \qquad \lambda_j = (\sum_{i\in\beta} \Delta_i^{(\beta)\prime})^{-1} \Delta_j^{(\beta)\prime},$$

where the primed determinants are evaluated at P'_β. Thus $P_\beta \in L_\beta$. However, $P_\beta \notin L_\gamma$ when γ is a proper subset of β, as

$$\mathbf{p}_\gamma^2 = 1 - \lambda^2(\mathbf{p}_\gamma'^2 - \mathbf{p}_\beta'^2) < 1 \quad \text{at} \quad P_\beta, \quad \text{by} \quad (3.6).$$

By choosing $\lambda_\beta^{(1)}$ so that P'_β is sufficiently close to L_β but far from the L_γ with $\gamma \not\subset \beta$ and by taking a sufficiently small value of λ, we can ensure that $\lambda_\beta^{(2)}$ does not intersect any L_γ with $\gamma \not\subset \beta$. The combined path λ_β will then meet all the requirements set out in Sec. 2.

We must now extend the definition of e_β to the whole of λ_β. As it is already defined on $\lambda_\beta^{(1)}$, we need only specify it on $\lambda_\beta^{(2)}$. Here we put $e_\beta = e_\beta^{(1)} + e_\beta^{(2)}$, where $e_\beta^{(1)}$ is given by (3.7) with

$$\pi_\beta = \{t + (1 - t)\eta\}^{-1}\mathbf{q}, \tag{3.18}$$

$e_\beta^{(2)}$ is zero if $|\beta| = 1$, and $|e_\beta^{(2)}|$ is defined for $|\beta| > 1$ to be the closure of the set of all $\mathbf{z}$ in $\mathbf{C}^{l+1}$ of the form

$$\mathbf{z} = \frac{\zeta}{\zeta^2} + i\left(\pi_\beta^2 - \frac{1}{\zeta^2}\right)^{-\frac{1}{2}}\left(\frac{1}{\zeta^2} - 1\right)^{\frac{1}{2}}\left(\frac{\zeta}{\zeta^2} - \pi_\beta\right) \tag{3.19}$$

with π_β given by (3.18), where

$$\zeta = (1 - t)\xi + t\mathbf{q} + i\lambda t(\mathbf{p}'_\beta - \xi) \tag{3.20}$$

and ξ is a real $(l + 1)$-vector belonging to the set E defined by

$$\mathbf{p}'_\beta\cdot\xi = (\mathbf{p}'_\beta)^2, \quad \xi \neq \mathbf{p}'_\beta, \mathbf{p}'_j\cdot\xi \geq \xi^2 \quad \text{for some} \quad j \in \beta. \tag{3.21}$$

The above conditions clearly define (to within orientation) a chain e_β of Σ whose boundary belongs to ${}_{(\beta)}\Sigma$, and this definition agrees at $P'_\beta(t = 0)$ with the previous definition of e_β at standard points. It remains only to show that e_β shrinks down to the point $\mathbf{z} = \mathbf{q}$ as $t \to 1$. Now $e_\beta^{(1)}$ clearly does have this "vanishing" property. Also $\pi_\beta \to \mathbf{q}$ as $t \to 1$. It is therefore sufficient to show that

$$\mathbf{z} - \pi_\beta = \left[1 + i\left(\pi_\beta^2 - \frac{1}{\zeta^2}\right)^{-\frac{1}{2}}\left(\frac{1}{\zeta^2} - 1\right)^{\frac{1}{2}}\right]\left(\frac{\zeta}{\zeta^2} - \pi_\beta\right) \tag{3.22}$$

with ζ given by (3.20) tends to zero as $t \to 1$ uniformly in ξ for ξ in E. For this purpose, it is convenient to rewrite (3.22) in the form

$$\mathbf{z} - \pi_\beta = (1 - \mathbf{p}_\beta^2)[(\zeta^2 - \mathbf{p}_\beta^2)^{\frac{1}{2}} - i\,|\mathbf{p}_\beta|\,(1 - \zeta^2)^{\frac{1}{2}}]^{-1} \times (\zeta^2 - \mathbf{p}_\beta^2)^{-\frac{1}{2}}(\zeta - \zeta^2\pi_\beta), \quad (3.23)$$

to put

$$\tau = 1 - t \quad (3.24)$$

and to investigate the behavior of (3.23) as $\tau \to 0$. We shall obtain an upper bound on $|\mathbf{z} - \pi_\beta|^2$ for $\xi \in E$ which tends to zero as $\tau \to 0$, where $|\mathbf{a}|^2$ for a complex vector $\mathbf{a}$ stands for the scalar product of $\mathbf{a}$ with its complex conjugate. A simple calculation shows that

$$\begin{aligned}|\zeta^2 - \mathbf{p}_\beta^2|^{-1}\,|\zeta - \zeta^2\pi_\beta|^2 &= 1 + (1 - \tau + \tau\eta)^{-2}[\lambda^2(1 - \tau)^2 + \tau^2](\xi^2 - \eta^2) \\ &< 1 + (1 - \tau + \tau\eta)^{-2}[\lambda^2(1 - \tau)^2 + \tau^2](1 - \eta^2).\end{aligned} \quad (3.25)$$

Also,

$$\begin{aligned}(\zeta^2 - \mathbf{p}_\beta^2)^{\frac{1}{2}} - i\,|\mathbf{p}_\beta|\,(1 - \zeta^2)^{\frac{1}{2}} &= -i\{Z + (1 - \tau + \tau\eta) \\ &\quad \times [\tau(1 - \eta)(2 - \tau + \tau\eta) + Z^2]^{\frac{1}{2}}\},\end{aligned} \quad (3.26)$$

where

$$Z = [\lambda + i(1 + i\lambda)\tau](\xi^2 - \eta^2)^{\frac{1}{2}}. \quad (3.27)$$

For τ sufficiently small, $0 \leq \arg Z \leq \frac{1}{4}\pi$ independently of ξ. Hence

$$\operatorname{Re}\{[\tau(1 - \eta)(2 - \tau + \tau\eta) + Z^2]^{\frac{1}{2}}\} \geq [\tau(1 - \eta)(2 - \tau + \tau\eta)]^{\frac{1}{2}}$$

so that

$$|(\zeta^2 - \mathbf{p}_\beta^2)^{\frac{1}{2}} - i\,|\mathbf{p}_\beta|\,(1 - \zeta^2)^{\frac{1}{2}}| \geq (1 - \tau + \tau\eta)[\tau(1 - \eta)(2 - \tau + \tau\eta)]^{\frac{1}{2}},$$

and

$$|(1 - \mathbf{p}_\beta^2)[(\zeta^2 - \mathbf{p}_\beta^2)^{\frac{1}{2}} - i\,|\mathbf{p}_\beta|\,(1 - \zeta^2)^{\frac{1}{2}}]^{-1}|^2 \leq (1 - \tau + \tau\eta)^{-2}\tau(1 - \eta)(2 - \tau + \tau\eta). \quad (3.28)$$

Thus, $|\mathbf{z} - \pi_\beta|^2$ cannot exceed the product of the right-hand sides of (3.25) and (3.28), a quantity which tends to zero as $\tau \to 0$.

4. EVALUATION OF KRONECKER INDICES

Before giving the orientations of the chains $e_\beta^{(1)}$ and $e_\beta^{(2)}$ at a standard point, we make some general remarks about the orientation of differentiable manifolds (in general manifolds with boundary) embedded in $\mathbf{R}^n$. Let M be a connected orientable m-dimensional differentiable manifold in $\mathbf{R}^n$ $(0 < m < n)$, and let $\mathbf{x}_0$ be any point of M. There are only two possible orientations for M. For a given local coordinate system $(x_1, \cdots x_m)$ is the neighborhood of $\mathbf{x}_0$, these two orientations will take the values 1 and -1 respectively. That which takes the value 1 will be called the orientation determined by the local coordinate system $(x_1, \cdots, x_m)$. Two local coordinate systems $(x_1, \cdots, x_m)$ and $(x_1', \cdots, x_m')$ in the neighborhood of $\mathbf{x}_0$ determine equal or opposite orientations according as the Jacobian

$$\partial(x_1', \cdots, x_m')/\partial(x_1, \cdots, x_m)$$

is positive or negative.

An ordered set of m vectors $\mathbf{e}_1, \cdots, \mathbf{e}_m$ of $\mathbf{R}^n$, whose (orthogonal) projections $\hat{\mathbf{e}}_1, \cdots, \hat{\mathbf{e}}_m$ onto the tangent m-plane T to M at $\mathbf{x}_0$ are linearly independent, determines an orientation of M, namely that determined by the local coordinate system $(\mathbf{e}_1 \cdot \mathbf{x}, \cdots, \mathbf{e}_m \cdot \mathbf{x})$ in the neighborhood of $\mathbf{x}_0$. This will be called the orientation determined by $\mathbf{e}_1, \cdots, \mathbf{e}_m$ at $\mathbf{x}_0$. Two sets of vectors $\{\mathbf{e}_1, \cdots, \mathbf{e}_m\}$ and $\{\mathbf{e}_1', \cdots, \mathbf{e}_m'\}$ determine equal or opposite orientations according as $\det(\hat{\mathbf{e}}_i \cdot \mathbf{e}_j')$ is positive or negative. In the special case where $\{\mathbf{e}_1, \cdots, \mathbf{e}_m\}$ and $\{\mathbf{e}_1', \cdots \mathbf{e}_m'\}$ span the same m-dimensional subspace of $\mathbf{R}^n$ (not necessarily T), the orientations determined by them at $\mathbf{x}_0$ will be equal or opposite according as $\det(\mathbf{e}_i \cdot \mathbf{e}_j')$ is positive or negative.

In the sequel we shall make repeated use of the relations

$$\det(\mathbf{a}_1, \cdots, \mathbf{a}_m, \mathbf{b}_{m+1}, \cdots, \mathbf{b}_n)\det(\mathbf{a}_1, \cdots, \mathbf{a}_m, \mathbf{b}_{m+1}', \cdots, \mathbf{b}_n') = \det(\mathbf{a}_i \cdot \mathbf{a}_j)\det(\mathbf{b}_k \cdot \mathbf{b}_l'), \quad (4.1)$$

$$\det(\mathbf{a}_1, \cdots, \mathbf{a}_m, \mathbf{b}_{m+1}', \cdots, \mathbf{b}_n')\det(\mathbf{a}_1', \cdots, \mathbf{a}_m', \mathbf{b}_{m+1}', \cdots, \mathbf{b}_n') = \det(\mathbf{a}_i \cdot \mathbf{a}_j')\det(\mathbf{b}_k' \cdot \mathbf{b}_l'), \quad (4.2)$$

which hold when the real n-vectors $\mathbf{a}_1, \cdots, \mathbf{a}_m, \mathbf{a}_1', \cdots, \mathbf{a}_m', \mathbf{b}_{m+1}, \cdots, \mathbf{b}_n, \mathbf{b}_{m+1}', \cdots, \mathbf{b}_n'$ are such that each $\mathbf{a}_i$ is orthogonal to each $\mathbf{b}_k$ and each $\mathbf{a}_i'$ is orthogonal to each $\mathbf{b}_k'$. Here, $\det(\mathbf{a}_1, \cdots, \mathbf{a}_m, \mathbf{b}_{m+1}, \cdots, \mathbf{b}_n)$, for example, means the determinant of the $n \times n$ matrix whose columns are $\mathbf{a}_1, \cdots, \mathbf{a}_m$,

$\mathbf{b}_{m+1}, \cdots, \mathbf{b}_n$. The proof of (4.1) and (4.2) is a straightforward application of the identities

$$\det(A) = \det(A^t),$$
$$\det(A)\det(B) = \det(AB),$$

where A and B are $n \times n$ matrices and A^t is the transpose of A.

Now the subset $|e_\beta^{(1)}|$ of $\mathbf{C}^{l+1}$ defined by (3.7) is an l-dimensional differentiable manifold with boundary. We give it the orientation determined by the global coordinate system $(\mathbf{e}_1\cdot\mathbf{y}, \cdots, \mathbf{e}_l\cdot\mathbf{y})$ where $\{\mathbf{e}_1, \cdots, \mathbf{e}_l\}$ is an orthonormal set of real vectors orthogonal to π_β and such that $\det(\pi_\beta, \mathbf{e}_1, \cdots, \mathbf{e}_l) > 0$. Clearly, any two such orthonormal sets determine the same orientation of $|e_\beta^{(1)}|$. The oriented manifold determines an l-chain of Σ which, by definition, is $e_\beta^{(1)}$. In terms of the given coordinate system, $|e_\beta^{(1)}|$ is given by

$$(\mathbf{e}_1\cdot\mathbf{y})^2 + (\mathbf{e}_2\cdot\mathbf{y})^2 + \cdots + (\mathbf{e}_l\cdot\mathbf{y})^2 \leq \pi_\beta^2 - 1, \quad (4.3)$$

and it is diffeomorphic to a closed l-ball. Its boundary is the $(l-1)$-sphere

$$\mathbf{x} = \pi_\beta, \qquad \pi_\beta\cdot\mathbf{y} = 0,$$
$$(\mathbf{e}_1\cdot\mathbf{y})^2 + \cdots + (\mathbf{e}_l\cdot\mathbf{y})^2 = \pi_\beta^2 - 1. \quad (4.4)$$

The orientation of the boundary induced by that of $|e_\beta^{(1)}|$ is clearly that determined by the local coordinate system $(\mathbf{e}_2\cdot\mathbf{y}, \cdots, \mathbf{e}_l\cdot\mathbf{y})$ in the neighborhood of the point

$$\mathbf{x} = \pi_\beta, \qquad \mathbf{y} = \mathbf{e}_1(\pi_\beta^2 - 1)^{\frac{1}{2}}. \quad (4.5)$$

This oriented boundary determines the cycle $\partial e_\beta^{(1)}$.

The set $|e_\beta^{(2)}|$ defined by (3.8) is a subset of the differentiable l-manifold with boundary M, defined as the subset of $\mathbf{C}^{l+1}$ in which either

$$\mathbf{x} = \pi_\beta, \qquad \pi_\beta\cdot\mathbf{y} = 0, \qquad \mathbf{y}^2 = \pi_\beta^2 - 1, \quad (4.6)$$

or

$$\mathbf{x}\cdot(\pi_\beta - \mathbf{x}) = 0, \qquad \mathbf{x}^2 > 1, \qquad \mathbf{x} \neq \pi_\beta,$$
$$\mathbf{y} = (\mathbf{x}^2 - 1)^{\frac{1}{2}}\,|\mathbf{x} - \pi_\beta|^{-1}(\mathbf{x} - \pi_\beta). \quad (4.7)$$

Let $\{\mathbf{e}_1, \cdots, \mathbf{e}_l\}$ be as in the definition of $e_\beta^{(1)}$. Then $(\mathbf{e}_1\cdot\mathbf{y}, \cdots, \mathbf{e}_l\cdot\mathbf{y})$ provides a global coordinate system for M and we give M the orientation *opposite* to that determined by this coordinate system. The orientation of $e_\beta^{(2)}$ is now defined to be that induced by the above orientation of M. The points of M all satisfy

$$0 < (\mathbf{e}_1\cdot\mathbf{y})^2 + \cdots + (\mathbf{e}_l\cdot\mathbf{y})^2 \leq \pi_\beta^2 - 1, \quad (4.8)$$

and its boundary ∂M is given by (4.4) or (4.6). Clearly ∂M has the orientation opposite to that of $\partial e_\beta^{(1)}$. Since $\partial e_\beta^{(2)}$ contains the whole of ∂M, it follows that $\partial e_\beta^{(1)}$ is canceled out in the sum and does not appear in ∂e_β.

It is generally more convenient to give the orientation of M, and hence of $e_\beta^{(2)}$, in terms of $\mathbf{x}$ rather than $\mathbf{y}$. Let us identify $\mathbf{C}^{l+1}$ with $\mathbf{R}^{2l+2}$ by the correspondence

$$z = \mathbf{x} + i\mathbf{y} \leftrightarrow \mathbf{X} = (\mathbf{x}, \mathbf{y}).$$

Suppose $\mathbf{X}_0 = (\mathbf{x}_0, \mathbf{y}_0)$ is a point of $M - \partial M$, and $\{\mathbf{a}_1, \cdots, \mathbf{a}_l\}$ a set of real $(l+1)$-vectors orthogonal to $2\mathbf{x}_0 - \pi_\beta$ such that

$$\det(2\mathbf{x}_0 - \pi_\beta, \mathbf{a}_1, \cdots, \mathbf{a}_l) > 0.$$

We show that the orientation of M determined at $\mathbf{X}_0$ by the $(2l+2)$-vectors $\mathbf{A}_1, \cdots, \mathbf{A}_l$ defined by $\mathbf{A}_i = (\mathbf{a}_i, \mathbf{0})$ is independent of the choice of the set $\{\mathbf{a}_1, \cdots, \mathbf{a}_l\}$. For let $\{\mathbf{a}_1', \cdots, \mathbf{a}_l'\}$ be another possible choice and put $\mathbf{A}_i' = (\mathbf{a}_i', \mathbf{0})$. As $\{\mathbf{A}_1, \cdots, \mathbf{A}_l\}$ and $\{\mathbf{A}_1', \cdots, \mathbf{A}_l'\}$ span the same l-dimensional subspace of $\mathbf{R}^{2l+2}$ we need only show that $\det(\mathbf{A}_i\cdot\mathbf{A}_j') = \det(\mathbf{a}_i\cdot\mathbf{a}_j')$ is positive. But (4.1) gives

$$\det(2\mathbf{x}_0 - \pi_\beta, \mathbf{a}_1, \cdots, \mathbf{a}_l)\det(2\mathbf{x}_0 - \pi_\beta, \mathbf{a}_1', \cdots, \mathbf{a}_l') = (2\mathbf{x}_0 - \pi_\beta)^2\det(\mathbf{a}_i\cdot\mathbf{a}_j'),$$

and, since the left-hand side is, by hypothesis, positive, it follows that $\det(\mathbf{a}_i\cdot\mathbf{a}_j')$ is positive. Thus the orientation of M determined at $\mathbf{X}_0$ by $\mathbf{A}_1, \cdots, \mathbf{A}_l$ is independent of the choice of $\mathbf{a}_1, \cdots, \mathbf{a}_l$. It is also clear, by considering overlapping neighborhoods, that this orientation is independent of the point $\mathbf{X}_0$. We now show that this orientation is in fact the same as that already defined for M, i.e., it is opposite to that determined by the global coordinate system $(\mathbf{e}_1\cdot\mathbf{y}, \cdots, \mathbf{e}_l\cdot\mathbf{y})$. To do this, we shall pick a particular point $\mathbf{X}_0$ in $M - \partial M$, and a particular set of $\mathbf{a}_i$, and show that $\det(\hat{\mathbf{A}}_i\cdot\mathbf{E}_j) < 0$, where $\mathbf{E}_j = (\mathbf{0}, \mathbf{e}_j)$. If $\mathbf{X}_0 = (\mathbf{x}_0, \mathbf{y}_0)$, we define, for every vector $\mathbf{v}$ of $\mathbf{R}^{l+1}$ orthogonal to $2\mathbf{x}_0 - \pi_\beta$,

$$\tilde{\mathbf{v}} = (\mathbf{x}_0^2 - 1)^{\frac{1}{2}}\,|\mathbf{x}_0 - \pi_\beta|^{-1}\mathbf{v}$$
$$- (\mathbf{x}_0^2 - 1)^{-\frac{1}{2}}\,|\mathbf{x}_0 - \pi_\beta|^{-3}(\pi_\beta^2 - 1)$$
$$\times [\mathbf{v}\cdot(\mathbf{x}_0 - \pi_\beta)](\mathbf{x}_0 - \pi_\beta). \quad (4.9)$$

Then

$$\hat{\mathbf{A}}_i = (\mathbf{a}_i^2 + \tilde{\mathbf{a}}_i^2)^{-1}\mathbf{a}_i^2(\mathbf{a}_i, \tilde{\mathbf{a}}_i). \quad (4.10)$$

It is therefore sufficient to show that $\det(\tilde{\mathbf{a}}_i \cdot \mathbf{e}_j) < 0$. We now make the choice

$$\mathbf{x}_0 = \pi_\beta \cos^2\alpha + \mathbf{e}_1 |\pi_\beta| \sin\alpha \cos\alpha,$$
$$\mathbf{y}_0 = (\mathbf{x}_0^2 - 1)^{\frac{1}{2}} |\mathbf{x}_0 - \pi_\beta|^{-1} (\mathbf{x}_0 - \pi_\beta),$$
$$\mathbf{a}_1 = \mathbf{e}_1 \cos 2\alpha - |\pi_\beta|^{-1} \pi_\beta \sin 2\alpha,$$
$$\mathbf{a}_i = \mathbf{e}_i, \quad \text{for} \quad i = 2, 3, \cdots, l,$$

where $0 < \alpha < \cos^{-1}(|\pi_\beta|^{-1})$. A short calculation shows that

$$\tilde{\mathbf{a}}_1 = -|\pi_\beta|^{-2} (\pi_\beta^2 \cos^2\alpha - 1)^{-\frac{1}{2}} \times \{|\pi_\beta| \sin\alpha(2\pi_\beta^2 \cos^2\alpha - 1)\mathbf{e}_1 + \cos\alpha(\pi_\beta^2 \cos 2\alpha - 1)\pi_\beta\},$$
$$\tilde{\mathbf{a}}_i = (|\pi_\beta| \sin\alpha)^{-1}(\pi_\beta^2 \cos^2\alpha - 1)^{\frac{1}{2}}\mathbf{e}_i, \quad \text{for} \quad i = 2, 3, \cdots, l.$$

Hence,

$$\det(\tilde{\mathbf{a}}_i \cdot \mathbf{e}_j) = -|\pi_\beta|^{-l} (\sin\alpha)^{-(l-2)} \times (2\pi_\beta^2 \cos^2\alpha - 1)(\pi_\beta^2 \cos^2\alpha - 1)^{\frac{1}{2}l-1} < 0. \quad (4.11)$$

Now that e_β has been oriented, the orientations of the (relative) cycles obtained from it by repeated applications of boundary operators are completely determined. In order to evaluate the necessary Kronecker indices, we shall need to know the values which these orientations take in appropriate local coordinate systems.

First, we consider the orientations of the chains $\partial_j e_\beta$ ($j \in \beta$) which make up the boundary of e_β for the case $|\beta| > 1$. Let $\mathbf{X}_0 = (\mathbf{x}_0, \mathbf{y}_0)$ belong to the set $|\partial_j e_\beta|$ given by (3.9) but not to any $|\partial_i e_\beta|$ with $i \neq j$. The orientation of e_β is that determined by a local coordinate system in the neighborhood of the boundary point $\mathbf{X}_0$ of the form $(\mathbf{a}_1 \cdot \mathbf{x}, \cdots, \mathbf{a}_l \cdot \mathbf{x})$, where we choose

$$\mathbf{a}_1 = \pi_j - |\pi_\beta|^{-2} [\pi_j \cdot (2\mathbf{x}_0 - \pi_\beta)](2\mathbf{x}_0 - \pi_\beta),$$

and take $\mathbf{a}_2, \cdots, \mathbf{a}_l$ to be vectors of $\mathbf{R}^{l+1}$ orthogonal to both $2\mathbf{x}_0 - \pi_\beta$ and $\mathbf{a}_1$ and satisfying

$$\det(2\mathbf{x}_0 - \pi_\beta, \mathbf{a}_1, \cdots \mathbf{a}_l) > 0.$$

This is possible because $\mathbf{a}_1 \not\equiv \mathbf{0}$ (since $2\mathbf{x}_0 - \pi_\beta$ and π_j cannot be parallel). For $(\mathbf{x}, \mathbf{y})$ in e_β close to $\mathbf{X}_0$, we have

$$\pi_j \cdot (\mathbf{x} - \mathbf{x}_0) = \mathbf{a}_1 \cdot (\mathbf{x} - \mathbf{x}_0) - |\pi_\beta|^{-2} \times [\pi_j \cdot (2\mathbf{x}_0 - \pi_\beta)](\mathbf{x} - \mathbf{x}_0)^2 \geq 0. \quad (4.12)$$

Thus, in terms of the orthogonal projection e'_β of e_β onto the "real" subspace $\mathbf{y} = \mathbf{0}$ of $\mathbf{R}^{2l+2}$, we see that $\mathbf{A}_1$ is in the direction of the normal to $\partial e'_\beta$ at $(\mathbf{x}_0, \mathbf{0})$ lying in e'_β and pointing towards its interior, while $\mathbf{A}_2, \cdots, \mathbf{A}_l$ are tangent vectors to $\partial e'_\beta$ at $(\mathbf{x}_0, \mathbf{0})$. The orientation of $\partial_j e_\beta$ therefore takes the value -1 in the local coordinate system $(\mathbf{a}_2 \cdot \mathbf{x}, \cdots, \mathbf{a}_l \cdot \mathbf{x})$ in the neighborhood of $\mathbf{X}_0$. By (4.2) we have

$$\det(2\mathbf{x}_0 - \pi_\beta, \mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_l) \det(2\mathbf{x}_0 - \pi_\beta, \pi_j, \mathbf{a}_2, \cdots, \mathbf{a}_l) = \begin{vmatrix} (2\mathbf{x}_0 - \pi_\beta)^2, & 0 \\ \pi_j \cdot (2\mathbf{x}_0 - \pi_\beta), & \pi_j^2 - |\pi_\beta|^{-2} \{\pi_j \cdot (2\mathbf{x}_0 - \pi_\beta)\}^2 \end{vmatrix} \det(\mathbf{a}_i \cdot \mathbf{a}_k).$$

The right-hand side is positive because the Gram determinant is positive and the first factor equals $\pi_j^2(\pi_\beta^2 - \pi_j^2)$ which is positive by (3.6). Hence, we could equally well have imposed on $\mathbf{a}_2, \cdots, \mathbf{a}_l$ the condition that they be orthogonal to both $2\mathbf{x}_0 - \pi_\beta$ and π_j, and that

$$\det(2\mathbf{x}_0 - \pi_\beta, \pi_j, \mathbf{a}_2, \cdots, \mathbf{a}_l) > 0.$$

Next, we consider the general case of the chains $e^{i_1 \cdots i_s}{}_{i_{s+1} \cdots i_r}$, where $0 < s < r$, $s < l$, $\beta = \{i_1, \cdots, i_r\}$. Let $\mathbf{X}_0 = (\mathbf{x}_0, \mathbf{y}_0)$ be any point of the set $|e^{i_1 \cdots i_s}{}_{i_{s+1} \cdots i_r}|$ given by (3.10). Suppose the vectors $\mathbf{a}_{s+1}, \cdots, \mathbf{a}_l$ of $\mathbf{R}^{l+1}$ are orthogonal to

$$2\mathbf{x}_0 - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_s}$$

and that

$$\det(2\mathbf{x}_0 - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_s}, \mathbf{a}_{s+1}, \cdots, \mathbf{a}_l) > 0. \quad (4.13)$$

We shall prove that the orientation of $e^{i_1 \cdots i_s}{}_{i_{s+1} \cdots i_r}$ takes the value -1 in the local coordinate system $(\mathbf{a}_{s+1} \cdot \mathbf{x}, \cdots, \mathbf{a}_l \cdot \mathbf{x})$ in the neighborhood of $\mathbf{X}_0$. The proof is by induction on s. We have just shown that it holds for $s = 1$. Let us suppose that it holds for the chain $e^{i_1 \cdots i_{s-1}}{}_{i_s \cdots i_r}$, where $s > 1$. Before completing the proof, we introduce some convenient notations. If $\mathbf{b}_1, \cdots, \mathbf{b}_m$ are linearly independent vectors of $\mathbf{R}^n$, we write $\Delta(\mathbf{b}_1, \cdots, \mathbf{b}_m)$ for the Gram determinant $\det(\mathbf{b}_i \cdot \mathbf{b}_j)$, which is necessarily positive.

If $\mathbf{c}$ is another vector of R^n, such that $\mathbf{b}_1, \cdots, \mathbf{b}_m, \mathbf{c}$ is linearly independent, we write

$$\mathbf{c}^{\perp}(\mathbf{b}_1, \cdots, \mathbf{b}_m) = [\Delta(\mathbf{b}_1, \cdots, \mathbf{b}_m)]^{-1} \begin{vmatrix} \mathbf{b}_1^2, & \mathbf{b}_1\cdot\mathbf{b}_2, & \cdots, & \mathbf{b}_1\cdot\mathbf{b}_m, & \mathbf{b}_1\cdot\mathbf{c} \\ \mathbf{b}_2\cdot\mathbf{b}_1, & \mathbf{b}_2^2, & \cdots, & \mathbf{b}_2\cdot\mathbf{b}_m, & \mathbf{b}_2\cdot\mathbf{c} \\ & & \cdots\cdots & & \\ \mathbf{b}_m\cdot\mathbf{b}_1, & \mathbf{b}_m\cdot\mathbf{b}_2, & \cdots, & \mathbf{b}_m^2, & \mathbf{b}_m\cdot\mathbf{c} \\ \mathbf{b}_1, & \mathbf{b}_2, & \cdots, & \mathbf{b}_m, & \mathbf{c} \end{vmatrix}$$

for the part of $\mathbf{c}$ orthogonal to $\mathbf{b}_1, \cdots, \mathbf{b}_m$. Let $\mathbf{X}_0 = (\mathbf{x}_0, \mathbf{y}_0)$ be a point of $e^{i_1\cdots i_s}{}_{i_{s+1}\cdots i_r}$, $\mathbf{a}_s = \pi_{i_s}^{\perp}(2\mathbf{x}_0 - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_{s-1}})$, and $\mathbf{a}_{s+1}, \cdots, \mathbf{a}_l$ vectors of R^{l+1} orthogonal to $2\mathbf{x}_0 - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_{s-1}}, \mathbf{a}_s$ such that

$$\det(2\mathbf{x}_0 - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_{s-1}}, \mathbf{a}_s, \mathbf{a}_{s+1}, \cdots, \mathbf{a}_l) > 0. \tag{4.14}$$

By the induction hypothesis, the orientation of $e^{i_1\cdots i_{s-1}}{}_{i_s\cdots i_r}$ takes the value -1 in the local coordinate system $(\mathbf{a}_s\cdot\mathbf{x}, \cdots, \mathbf{a}_l\cdot\mathbf{x})$ in the neighborhood of $\mathbf{X}_0$. The points $(\mathbf{x}, \mathbf{y})$ of $e^{i_1\cdots i_{s-1}}{}_{i_s\cdots i_r}$ close to $\mathbf{X}_0$ satisfy

$$\pi_{i_s}\cdot(\mathbf{x} - \mathbf{x}_0) = \mathbf{a}_s\cdot(\mathbf{x} - \mathbf{x}_0) - c(\mathbf{x} - \mathbf{x}_0)^2 \leq 0, \tag{4.15}$$

where c is independent of $\mathbf{x}$. Hence, taking note of the difference in sign between (4.12) and (4.15), we see that the orientation of $e^{i_1\cdots i_s}{}_{i_{s+1}\cdots i_r}$ takes the value -1 in the local coordinate system $(\mathbf{a}_{s+1}\cdot\mathbf{x}, \cdots, \mathbf{a}_l\cdot\mathbf{x})$ in the neighborhood of $\mathbf{X}_0$. By (4.2) we have

$$\det(2\mathbf{x}_0 - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_{s-1}}, \mathbf{a}_s, \mathbf{a}_{s+1}, \cdots, \mathbf{a}_l)\det(2\mathbf{x}_0 - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_s}, \mathbf{a}_{s+1}, \cdots, \mathbf{a}_l) = \Delta(2\mathbf{x}_0 - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_s})\,\Delta(\mathbf{a}_{s+1}, \cdots, \mathbf{a}_l) > 0.$$

Hence $\mathbf{a}_{s+1}, \cdots, \mathbf{a}_l$ satisfy (4.14) if (and only if) they satisfy (4.13). This completes the induction proof of the statement made at the beginning of this paragraph. The corresponding statement and its proof in the case, $s = l$, $r = l + 1$ (when $e^{i_1\cdots i_s}{}_{i_{s+1}\cdots i_r}$ reduces to a pair of points) are obvious modifications of the above.

Finally, we have to consider the orientation of the vanishing cycle $e^\beta = e^{i_1\cdots i_r} = \partial_{i_r} e^{i_1\cdots i_{r-1}}{}_{i_r}$. We consider only the case $r < l$, the modifications necessary in the case $r = l$ being obvious. Let $\{\mathbf{e}_r, \cdots, \mathbf{e}_l\}$ be an orthonormal set of vectors in R^{l+1} orthogonal to $\pi_{i_1}, \pi_{i_2}, \cdots, \pi_{i_r}$ and such that

$$\det(\pi_{i_1}, \cdots, \pi_{i_r}, \mathbf{e}_r, \mathbf{e}_{r+1}, \cdots, \mathbf{e}_l) > 0. \tag{4.16}$$

We show that the orientation of $e^{i_1\cdots i_r}$ takes the value $(-1)^{r-1}$ in the local coordinate system $(\mathbf{e}_{r+1}\cdot\mathbf{y}, \cdots, \mathbf{e}_l\cdot\mathbf{y})$ in the neighborhood of the point

$$\mathbf{x} = \pi_\beta, \qquad \mathbf{y} = \mathbf{e}_r(\pi_\beta^2 - 1)^{\frac{1}{2}}.$$

Our discussion of the orientation of $e_\beta^{(1)}$ and its boundary shows that this is the case when $r = |\beta| = 1$. We can therefore assume $r > 1$. Consider the point $\mathbf{X}_0 = (\mathbf{x}_0, \mathbf{y}_0)$ of $e^{i_1\cdots i_{r-1}}{}_{i_r}$ defined by

$$\mathbf{x}_0 = \pi_\gamma + (\pi_\beta - \pi_\gamma)\cos^2\alpha + \mathbf{e}_r\,|\pi_\beta - \pi_\gamma|\sin\alpha\cos\alpha,$$

$$\mathbf{y}_0 = (\mathbf{x}_0^2 - 1)^{\frac{1}{2}}\,|\mathbf{x}_0 - \pi_\beta|^{-1}(\mathbf{x}_0 - \pi_\beta),$$

where $\gamma = \{i_1, \cdots, i_{r-1}\}$ and α satisfies $0 < \alpha < \frac{1}{4}\pi$. Let us define

$$\mathbf{a}_r = \mathbf{e}_r\cos 2\alpha - |\pi_\beta - \pi_\gamma|^{-1}(\pi_\beta - \pi_\gamma)\sin 2\alpha,$$

$$\mathbf{a}_i = \mathbf{e}_i \quad \text{for} \quad i = r + 1, \cdots, l.$$

Then the $\mathbf{a}_i$ are all orthogonal to

$$2\mathbf{x}_0 - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_{r-1}}.$$

It follows by (4.1) that

$$\det(\pi_{i_1}, \cdots, \pi_{i_{r-1}}, 2\mathbf{x}_0 - \pi_\beta, \mathbf{a}_r, \cdots, \mathbf{a}_l)\det(\pi_{i_1}, \cdots, \pi_{i_{r-1}}, 2\mathbf{x}_0 - \pi_\beta, \mathbf{e}_r, \cdots, \mathbf{e}_l) = \Delta(\pi_{i_1}, \cdots, \pi_{i_{r-1}}, 2\mathbf{x}_0 - \pi_\beta)\cos 2\alpha,$$

and by (4.2) that

$$\det(\pi_{i_1}, \cdots, \pi_{i_r}, \mathbf{e}_r, \cdots, \mathbf{e}_l) \det(\pi_{i_1}, \cdots, \pi_{i_{r-1}}, 2\mathbf{x}_0 - \pi_\beta, \mathbf{e}_r, \cdots, \mathbf{e}_l)$$

$$= \begin{vmatrix} \pi_{i_1}^2, & \pi_{i_1}\cdot\pi_{i_2}, & \cdots, & \pi_{i_1}\cdot\pi_{i_{r-1}}, & \pi_{i_1}\cdot(2\mathbf{x}_0 - \pi_\beta) \\ \vdots & \cdots\cdots & & \vdots & \vdots \\ \vdots & \cdots\cdots & & \vdots & \vdots \\ \pi_{i_{r-1}}\cdot\pi_{i_1}, & \cdots\cdots, & & \pi_{i_{r-1}}^2, & \pi_{i_{r-1}}\cdot(2\mathbf{x}_0 - \pi_\beta) \\ \pi_{i_r}\cdot\pi_{i_1}, & \cdots\cdots, & & \pi_{i_r}\cdot\pi_{i_{r-1}}, & \pi_{i_r}\cdot(2\mathbf{x}_0 - \pi_\beta) \end{vmatrix}$$

$$= \begin{vmatrix} \pi_{i_1}^2, & \pi_{i_1}\cdot\pi_{i_2}, & \cdots, & \pi_{i_1}\cdot\pi_{i_{r-1}}, & \pi_{i_1}\cdot\pi_\gamma \\ \vdots & \cdots\cdots & & \vdots & \vdots \\ \vdots & \cdots\cdots & & \vdots & \vdots \\ \pi_{i_{r-1}}\cdot\pi_{i_1}, & \cdots\cdots, & & \pi_{i_{r-1}}^2, & \pi_{i_{r-1}}\cdot\pi_\gamma \\ \pi_{i_r}\cdot\pi_{i_1}, & \cdots\cdots, & & \pi_{i_r}\cdot\pi_{i_{r-1}}, & \pi_{i_r}\cdot\pi_\gamma + (\pi_{i_r}^2 - \pi_{i_r}\cdot\pi_\gamma)\cos 2\alpha \end{vmatrix}$$

$$= \Delta(\pi_{i_1}, \cdots, \pi_{i_{r-1}})(\pi_{i_r}^2 - \pi_{i_r}\cdot\pi_\gamma)\cos 2\alpha,$$

where we used in the last step the fact that π_γ is a linear combination of $\pi_{i_1}, \cdots, \pi_{i_{r-1}}$. Since $\pi_{i_r}^2 - \pi_{i_r}\cdot\pi_\gamma > 0$ by (3.12) and the Gram determinants are positive, it follows from (4.16) that

$$\det(\pi_{i_1}, \cdots, \pi_{i_{r-1}}, 2\mathbf{x}_0 - \pi_\beta, \mathbf{a}_r, \cdots, \mathbf{a}_l) = (-1)^{r-1}\det(2\mathbf{x}_0 - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_{r-1}}, \mathbf{a}_r, \cdots, \mathbf{a}_l) > 0.$$

We conclude that the orientation of $e^{i_1\cdots i_{r-1}}{}_{i_r}$ takes the value $(-1)^r$ in the local coordinate system $(\mathbf{a}_r\cdot\mathbf{x}, \mathbf{a}_{r+1}\cdot\mathbf{x}, \cdots, \mathbf{a}_l\cdot\mathbf{x})$ in the neighborhood of $\mathbf{X}_0$. From (4.9) we find after some reduction that

$$\tilde{\mathbf{a}}_r = -|\pi_\beta - \pi_\gamma|^{-2}[\pi_\gamma^2 + (\pi_\beta - \pi_\gamma)^2\cos^2\alpha - 1]^{-\frac{1}{2}}$$
$$\times \{|\pi_\beta - \pi_\gamma|\sin\alpha[\pi_\beta^2 + (\pi_\beta - \pi_\gamma)^2\cos 2\alpha - 1]\mathbf{e}_r + \cos\alpha[\pi_\beta^2 - 2(\pi_\beta - \pi_\gamma)^2\sin^2\alpha - 1](\pi_\beta - \pi_\gamma)\},$$

$$\tilde{\mathbf{a}}_i = (|\pi_\beta - \pi_\gamma|\sin\alpha)^{-1}[\pi_\gamma^2 + (\pi_\beta - \pi_\gamma)^2\cos^2\alpha - 1]^{\frac{1}{2}}\mathbf{e}_i, \quad \text{for} \quad i = r+1, \cdots, l,$$

whence it is easy to show that $\det(\tilde{\mathbf{a}}_i\cdot\mathbf{e}_j)$ is negative. The orientation of $e^{i_1\cdots i_{r-1}}{}_{i_r}$ therefore takes the value $(-1)^{r-1}$ in the local coordinate system $(\mathbf{e}_r\cdot\mathbf{y}, \mathbf{e}_{r+1}\cdot\mathbf{y}, \cdots, \mathbf{e}_l\cdot\mathbf{y})$ in the neighborhood of $\mathbf{X}_0$. But, by choosing α small enough, we can make $\mathbf{X}_0$ arbitrarily close to the point $\mathbf{X}_1$ of e^β defined by

$$\mathbf{X}_1 = (\mathbf{x}_1, \mathbf{y}_1); \mathbf{x}_1 = \pi_\beta, \qquad \mathbf{y}_1 = \mathbf{e}_r(\pi_\beta^2 - 1)^{\frac{1}{2}}.$$

Hence, the orientation of $e^{i_1\cdots i_{r-1}}{}_{i_r}$ takes the value $(-1)^{r-1}$ in the local coordinate system $(\mathbf{e}_r\cdot\mathbf{y}, \mathbf{e}_{r+1}\cdot\mathbf{y}, \cdots, \mathbf{e}_l\cdot\mathbf{y})$ in the neighborhood of $\mathbf{X}_1$. As the points of $e^{i_1\cdots i_{r-1}}{}_{i_r}$ close to $\mathbf{X}_1$ satisfy

$$(\mathbf{e}_r\cdot\mathbf{y})^2 + (\mathbf{e}_{r+1}\cdot\mathbf{y})^2 + \cdots + (\mathbf{e}_l\cdot\mathbf{y})^2 \leq \pi_\beta^2 - 1,$$

it follows that the orientation of $e^{i_1\cdots i_r}$ takes the value $(-1)^{r-1}$ in the local coordinate system $(\mathbf{e}_{r+1}\cdot\mathbf{y}, \cdots, \mathbf{e}_l\cdot\mathbf{y})$ in the neighborhood of $\mathbf{X}_1$.

We are now in a position to evaluate the various Kronecker indices that will be needed in Sec. 5. First, let us recall the definition of the Kronecker index for chains of the special type we have been considering.[5] The Kronecker index KI $[c_1, c_2]$ of a p-chain c_1 with a q-chain c_2 in a differentiable manifold M of dimension $n = p + q$ is only defined when c_1 and c_2 have a finite number of points of intersection. In the neighborhood of a point of intersection P, we can find a local coordinate system $(x_1, \cdots, x_n)$ for M such that c_1 is given locally by $x_{p+1} = \cdots = x_n = 0$ and c_2 by $x_1 = \cdots = x_p = 0$. Let ϵ_1, ϵ_2, and ϵ be the values of the orientations of c_1, c_2, and M in the local coordinate systems $(x_1, \cdots, x_p)$, $(x_{p+1}, \cdots, x_n)$, and $(x_1, \cdots, x_n)$ respectively. The orientations of c_1 and c_2 will be said to agree or to disagree at P according as $\epsilon_1\epsilon_2 = \epsilon$ or $\epsilon_1\epsilon_2 = -\epsilon$. The Kronecker index KI $[c_1, c_2]$ is defined to be the number of points of intersection at which the orientations of c_1 and c_2 agree minus the number at which they disagree.

Consider first the Kronecker index KI $[\bar{\Gamma}, e_\beta]$, where $\beta \in B$. It is clear that $\bar{\Gamma}$ and e_β have only one point in common, namely the point

$$\mathbf{x} = |\pi_\beta|^{-1}\pi_\beta, \qquad \mathbf{y} = 0 \tag{4.17}$$

of $\mathbf{C}^{l+1}$, which belongs to $e_\beta^{(1)}$. Let $\{\mathbf{e}_1, \cdots, \mathbf{e}_l\}$ be an orthonormal set of vectors in $\mathbf{R}^{l+1}$ orthogonal to π_β, such that

$$\det(\pi_\beta, \mathbf{e}_1, \cdots, \mathbf{e}_l) > 0.$$

[5] G. de Rham, *Variétés différentiables* (Hermann & Cie., Paris, 1960).

Then the orientation of Γ takes the value 1 in the local coordinate system $(\mathbf{e}_1\cdot\mathbf{x}, \cdots, \mathbf{e}_l\cdot\mathbf{x})$ in the neighborhood of the point (4.17), while that of $e_\beta^{(1)}$ takes the value 1 in the coordinate system $(\mathbf{e}_1\cdot\mathbf{y}, \cdots, \mathbf{e}_l\cdot\mathbf{y})$. Moreover, the points of Γ satisfy $\mathbf{e}_i\cdot\mathbf{y} = 0$ $(i = 1, \cdots, l)$, while the points of e_β close to (4.17) satisfy $\mathbf{e}_i\cdot\mathbf{x} = 0$ $(\mathbf{y}^2)$ $(i = 1, \cdots, l)$. But the canonical orientation of the complex analytic manifold $\overline{\Sigma}$ takes the value 1 in the (real) local coordinate system

$$(\mathbf{e}_1\cdot\mathbf{x}, \mathbf{e}_1\cdot\mathbf{y}, \mathbf{e}_2\cdot\mathbf{x}, \mathbf{e}_2\cdot\mathbf{y}, \cdots, \mathbf{e}_l\cdot\mathbf{x}, \mathbf{e}_l\cdot\mathbf{y}),$$

and therefore takes the value $(-1)^{(1/2)l(l-1)}$ in the local coordinate system

$$(\mathbf{e}_1\cdot\mathbf{x}, \mathbf{e}_2\cdot\mathbf{x}, \cdots, \mathbf{e}_l\cdot\mathbf{x}, \mathbf{e}_1\cdot\mathbf{y}, \mathbf{e}_2\cdot\mathbf{y}, \cdots, \mathbf{e}_l\cdot\mathbf{y}).$$

We conclude at once that

$$\mathrm{KI}\,[\Gamma, e_\beta] = (-1)^{\frac{1}{2}l(l-1)}. \tag{4.18}$$

The other Kronecker indices that we have to evaluate are those of the form $\mathrm{KI}\,[\delta^{|\gamma|}e^\gamma, e_\beta]$, where $\beta, \gamma \in B$. It follows from the duality of boundary and coboundary operators with respect to the Kronecker index that

$$\mathrm{KI}\,[\delta^{|\gamma|}\,e^\gamma, e_\beta] = \mathrm{KI}\,[e^\gamma, \partial^{|\gamma|}\,e_\beta].$$

More precisely, if $\gamma = \{i_1, \cdots, i_s\}$, we have the relation

$$\mathrm{KI}\,[\delta_{i_1}\cdots\delta_{i_s}\,e^{i_1\cdots i_s}, e_\beta] = \mathrm{KI}\,[e^{i_1\cdots i_s}, \partial_{i_s}\cdots\partial_{i_1}\,e_\beta].$$

As the boundary of e_β is in ${}_{(\beta)}\overline{\Sigma}$, it follows at once that

$$\mathrm{KI}\,[\delta^{|\gamma|}\,e^\gamma, e_\beta] = 0, \quad \text{if} \quad \gamma \not\subset \beta. \tag{4.19}$$

For $\beta = \gamma$ we have

$$\mathrm{KI}\,[\delta^{|\beta|}\,e^\beta, e_\beta] = \mathrm{KI}\,[e^\beta, e^\beta]$$
$$= (-1)^{\frac{1}{2}(l-|\beta|)(l-|\beta|+1)} + (-1)^{\frac{1}{2}(l-|\beta|)(l-|\beta|-1)} \tag{4.20}$$

by Cartan's formula for the Kronecker indices of hyperspheres.[6]

There remains now only the case in which γ is a proper subset of β. Suppose $\beta = \{i_1, \cdots, i_r\}$, $\gamma = \{i_1, \cdots, i_s\}$, where $0 < s < r$. We have to find the Kronecker index

$$\mathrm{KI}\,[\delta^{|\gamma|}\,e^\gamma, e_\beta] = \mathrm{KI}\,[e^{i_1\cdots i_s}, e^{i_1\cdots i_s}{}_{i_{s+1}\cdots i_r}].$$

Now $e^{i_1\cdots i_s}$ and $e^{i_1\cdots i_s}{}_{i_{s+1}\cdots i_r}$ have a single point in common, namely the point $\mathbf{X}_0 = (\mathbf{x}_0, \mathbf{y}_0)$, where

$$\mathbf{x}_0 = \pi_\gamma, \qquad \mathbf{y}_0 = (\pi_\gamma^2 - 1)^{\frac{1}{2}}\,|\pi_\gamma - \pi_\beta|^{-1}\,(\pi_\gamma - \pi_\beta).$$

Let $\{\mathbf{e}_{s+1}, \cdots, \mathbf{e}_l\}$ be an orthonormal set of vectors in $\mathbf{R}^{l+1}$ orthogonal to $\pi_{i_1}, \pi_{i_2}, \cdots, \pi_{i_s}, \pi_\gamma - \pi_\beta$ and satisfying

$$\det(\pi_{i_1}, \cdots, \pi_{i_s}, \pi_\gamma - \pi_\beta, \mathbf{e}_{s+1}, \cdots, \mathbf{e}_l) > 0.$$

By (4.2) it follows that

$$\begin{aligned}\det(2\pi_\gamma - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_s}, \mathbf{e}_{s+1}, \cdots \mathbf{e}_l)\,&\det(\pi_{i_1}, \cdots, \pi_{i_s}, \pi_\gamma - \pi_\beta, \mathbf{e}_{s+1}, \cdots, \mathbf{e}_l)\\ &= (-1)^s \det(2\pi_\gamma - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_s}, \mathbf{e}_{s+1}, \cdots, \mathbf{e}_l)\,\det(\pi_\gamma - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_s}, \mathbf{e}_{s+1}, \cdots, \mathbf{e}_l)\\ &= (-1)^s(\pi_\beta^2 - \pi_\gamma^2)\,\Delta(\pi_{i_1}, \cdots, \pi_{i_s}),\end{aligned}$$

whence

$$(-1)^s \det(2\pi_\gamma - \pi_\beta, \pi_{i_1}, \cdots, \pi_{i_s}, \mathbf{e}_{s+1}, \cdots, \mathbf{e}_l) > 0$$

since $\pi_\beta^2 > \pi_\gamma^2$ by (3.6). We define vectors $\mathbf{E}_i$, $\mathbf{F}_i$, and $\mathbf{F}_i'$ in $\mathbf{R}^{2l+2}$ by

$$\mathbf{E}_i = (\mathbf{e}_i, 0), \qquad \mathbf{F}_i = (0, \mathbf{e}_i),$$
$$\mathbf{F}_i' = (-\,|\pi_\gamma - \pi_\beta|^{-1}\,(\pi_\gamma^2 - 1)^{\frac{1}{2}}\,\mathbf{e}_i, \mathbf{e}_i)$$

for $i = s + 1, \cdots, l$. The orientation of $e^{i_1\cdots i_s}$ takes the value $(-1)^{s-1}$ in the local coordinate system $[\mathbf{F}_{s+1}\cdot(\mathbf{X} - \mathbf{X}_0), \cdots, \mathbf{F}_l\cdot(\mathbf{X} - \mathbf{X}_0)]$ and therefore also in the local coordinate system $[\mathbf{F}_{s+1}'\cdot(\mathbf{X} - \mathbf{X}_0), \cdots, \mathbf{F}_l'\cdot(\mathbf{X} - \mathbf{X}_0)]$ in the neighborhood of $\mathbf{X}_0$, since the $\mathbf{F}_i$ lie in the tangent $(l - s)$-plane to $e^{i_1\cdots i_s}$ at $\mathbf{X}_0$ and

$$\det(\mathbf{F}_i\cdot\mathbf{F}_j') = \det(\mathbf{e}_i\cdot\mathbf{e}_j) > 0.$$

The orientation of $e^{i_1\cdots i_s}{}_{i_{s+1}\cdots i_r}$ takes the value $(-1)^{s-1}$ in the local coordinate system

$$[\mathbf{E}_{s+1}\cdot(\mathbf{X} - \mathbf{X}_0), \cdots, \mathbf{E}_l\cdot(\mathbf{X} - \mathbf{X}_0)].$$

The points $\mathbf{X}$ of $e^{i_1\cdots i_s}$ satisfy

$$\mathbf{E}_i\cdot(\mathbf{X} - \mathbf{X}_0) = 0, \quad \text{for} \quad i = s + 1, \cdots, l,$$

while the points of $e^{i_1\cdots i_s}{}_{i_{s+1}\cdots i_r}$ close to $\mathbf{X}_0$ satisfy

$$\mathbf{F}_i'\cdot(\mathbf{X} - \mathbf{X}_0) = 0(|\mathbf{X} - \mathbf{X}_0|^2), \text{ for } i = s + 1, \cdots, l.$$

Now, the canonical orientation of ${}^{(\gamma)}\Sigma$ is that determined by the vectors

$$[\mathbf{E}_{s+1}, \mathbf{F}_{s+1}, \mathbf{E}_{s+2}, \mathbf{F}_{s+2}, \cdots, \mathbf{E}_l, \mathbf{F}_l]$$

[6] E. Cartan, *OEuvres complètes* (Gauthier-Villars, Paris, 1952), Pt. I, Vol. 2, p. 1227.

at $\mathbf{X}_0$. It therefore takes the value $(-1)^{(1/2)(l-s)(l-s+1)}$ in the local coordinate system

$$[\mathbf{F}_{s+1}\cdot(\mathbf{X}-\mathbf{X}_0), \cdots, \mathbf{F}_l\cdot(\mathbf{X}-\mathbf{X}_0), \mathbf{E}_{s+1}\cdot(\mathbf{X}-\mathbf{X}_0), \cdots, \mathbf{E}_l\cdot(\mathbf{X}-\mathbf{X}_0)],$$

and also, as may easily be verified, in the local coordinate system

$$[\mathbf{F}'_{s+1}\cdot(\mathbf{X}-\mathbf{X}_0), \cdots, \mathbf{F}'_l\cdot(\mathbf{X}-\mathbf{X}_0), \mathbf{E}_{s+1}\cdot(\mathbf{X}-\mathbf{X}_0), \cdots, \mathbf{E}_l\cdot(\mathbf{X}-\mathbf{X}_0)].$$

Therefore,

$$\mathrm{KI}\,[e^{i_1\cdots i_s}, e^{i_1\cdots i_s}{}_{i_{s+1}\cdots i_r}] = (-1)^{\frac{1}{2}(l-s)(l-s+1)}$$

so that

$$\mathrm{KI}\,[\delta^{|\gamma|}\,e^{\gamma}, e_\beta] = (-1)^{\frac{1}{2}(l-|\gamma|)(l-|\gamma|+1)}, \quad \text{when} \quad \gamma \subset \beta, \quad \gamma \neq \beta. \tag{4.21}$$

5. RELATIONS BETWEEN DISCONTINUITIES

It follows from the decomposition theorem of Fotiadi *et al.*[3] that, when the $\bar{\Sigma}_i$ are in general position in $\bar{\Sigma}$,

$$H_i^c\Big(\bar{\Sigma} - \bigcup_{j=1}^{m}\bar{\Sigma}_j\Big) \cong H_i^c\Big(\Sigma - \bigcup_{j=1}^{m-1}\Sigma_j\Big) \cong \bigoplus_{\beta\subset\{1,\cdots,m-1\}} \delta^{|\beta|}\, H^c_{l-|\beta|}({}^{(\beta)}\Sigma), \tag{5.1}$$

where the direct summation is over all subsets β of $\{1, \cdots, m-1\}$ (including the empty set $\varnothing$) and the iterated coboundary homomorphisms $\delta^{|\beta|}$ are all injective. The first isomorphism is that induced by the homeomorphism of $P^{l+1}(\mathbf{C}) - \bar{P}_m$ onto $\mathbf{C}^{l+1}$ obtained by treating $\bar{P}_m$ as hyperplane at infinity.

These isomorphisms hold in particular at any standard point, and may be used to obtain linear relations between the $\mathbf{e}_\beta$, where

$$\mathbf{e}_\beta = \delta^{|\beta|}\,e^\beta, \quad \text{for} \quad \beta \subset \{1, \cdots, m\}, \quad 1 \le |\beta| \le l, \tag{5.2}$$

$$\mathbf{e}_\varnothing = (-1)^l\bar{\Gamma}.$$

We consider first the case $m \le l$. As ${}^{(\beta)}\Sigma$ has the $(l-|\beta|)$-sphere as a deformation retract, it follows that each of the $H^c_{l-|\beta|}({}^{(\beta)}\Sigma)$ occurring in (5.1) is an infinite cyclic group. Hence, $H_i^c(\bar{\Sigma} - \bigcup_{i=1}^{m}\bar{\Sigma}_i)$ is a free Abelian group of rank 2^{m-1}, and the $\mathbf{e}_\beta$ with $\beta \subset \{1, \cdots, m-1\}$ form a basis for it. Now, the compact relative homology group $H_i^c(\bar{\Sigma}, \bigcup_{i=1}^{m}\bar{\Sigma}_i)$ is dual to the closed homology group $H_i^F(\bar{\Sigma} - \bigcup_{i=1}^{m}\bar{\Sigma}_i)$, and hence (since $\bar{\Sigma}$ is compact) to $H_i^c(\bar{\Sigma} - \bigcup_{i=1}^{m}\bar{\Sigma}_i)$, the duality being realized by the Kronecker index. Therefore, $H_i^c(\bar{\Sigma}, \bigcup_{i=1}^{m}\bar{\Sigma}_i)$ is also a free Abelian group of rank 2^{m-1} and has a basis $\{{}^\beta e\}$ dual to the basis $\{\mathbf{e}_\beta\}$ of $H_i^c(\bar{\Sigma} - \bigcup_{i=1}^{m}\bar{\Sigma}_i)$ in the sense that

$$\mathrm{KI}\,[\mathbf{e}_\beta, {}^\gamma e] = \delta_{\beta\gamma}, \quad \text{for} \quad \beta, \gamma \subset \{1, \cdots, m-1\}. \tag{5.3}$$

This dual basis is given by

$$\begin{aligned} {}^\beta e &= (-1)^{\frac{1}{2}(l-|\beta|)(l-|\beta|-1)}(e_\beta - e_{\beta m}), \\ &\text{for} \quad \beta \subset \{1, \cdots, m-1\}, \quad 1 \le |\beta| \le l, \\ {}^\varnothing e &= (-1)^{\frac{1}{2}l(l+1)}e_m, \end{aligned} \tag{5.4}$$

as may readily be verified using (4.18), (4.19), (4.20), and (4.21).

Since the $\mathbf{e}_\beta$ with $\beta \subset \{1, \cdots, m-1\}$ form a basis of $H_i^c(\bar{\Sigma} - \bigcup_{i=1}^{m}\bar{\Sigma}_i)$, the remaining $\mathbf{e}_\beta$ may be uniquely expressed as linear combinations of them. Thus, if $\gamma \subset \{1, \cdots, m-1\}$, there exist unique integers $n_{\beta\gamma}$ such that

$$\mathbf{e}_{\gamma m} = \sum_{\beta\subset\{1,\cdots,m-1\}} n_{\beta\gamma}\mathbf{e}_\beta. \tag{5.5}$$

On taking the Kronecker index of (5.5) with ${}^\beta e$ and applying (5.3), one finds that

$$n_{\beta\gamma} = \mathrm{KI}\,[\mathbf{e}_{\gamma m}, {}^\beta e].$$

Substituting from (5.4) and applying (4.18), (4.19), (4.20), and (4.21) we obtain finally the relations

$$\mathbf{e}_{\gamma m} = \{(-1)^{l-|\gamma|} - 1\}\mathbf{e}_\gamma - \sum_{\substack{\gamma\subset\beta\subset\{1,\cdots,m-1\}\\ \beta\neq\gamma}} (-1)^{\frac{1}{2}(|\beta|-|\gamma|)(2l-|\beta|-|\gamma|-1)}\mathbf{e}_\beta \tag{5.6}$$

for all $\gamma \subset \{1, \cdots, m-1\}$.

Now, the basis of $H_i^c(\bar{\Sigma} - \bigcup_{i=1}^{m}\bar{\Sigma}_i)$ consisting of the $\mathbf{e}_\beta$ with $\beta \subset \{1, \cdots, m-1\}$ determines a faithful representation of Aut $H_i^c(\bar{\Sigma} - \bigcup_{i=1}^{m}\bar{\Sigma}_i)$, in which each automorphism is represented by a non-singular $2^{m-1} \times 2^{m-1}$ matrix with integer elements. In particular, the automorphism ψ_β defined by (2.3) is represented by the matrix $A^{(\beta)}$, where

$$\psi_\beta(\mathbf{e}_\alpha) = \sum_{\gamma\subset\{1,\cdots,m-1\}} A^{(\beta)}_{\gamma\alpha}\mathbf{e}_\gamma, \quad \alpha \subset \{1, \cdots, m-1\}. \tag{5.7}$$

It is convenient to write

$$A^{(\beta)}_{\gamma\alpha} = \delta_{\gamma\alpha} + B^{(\beta)}_{\gamma\alpha}. \tag{5.8}$$

Applying (2.2), (2.3), (4.18), (4.19), (4.20), and

(4.21), we find that, for $\beta \subset \{1, \cdots, m-1\}$, $\beta \neq \varnothing$,

$$B^{(\beta)}_{\gamma\alpha} = 0, \quad \text{unless} \quad \alpha \subset \beta \quad \text{and} \quad \gamma = \beta,$$
$$B^{(\beta)}_{\beta\alpha} = -(-1)^{\frac{1}{2}(|\beta|-|\alpha|+1)(2l-|\beta|-|\alpha|)},$$
$$\text{when} \quad \alpha \subset \beta, \quad \alpha \neq \beta, \tag{5.9}$$
$$B^{(\beta)}_{\beta\beta} = -[1 + (-1)^{l-|\beta|}],$$

while

$$B^{(\beta m)}_{\gamma\alpha} = 0, \quad \text{unless} \quad \alpha \subset \beta \subset \gamma,$$
$$B^{(\beta m)}_{\gamma\alpha} = -(-1)^{\frac{1}{2}(|\gamma|-|\alpha|+1)(2l-|\gamma|-|\alpha|)}(-1)^{l-|\beta|}$$
$$\text{when} \quad \alpha \subset \beta \subset \gamma, \quad \gamma \neq \beta, \tag{5.10}$$
$$B^{(\beta m)}_{\beta\alpha} = (-1)^{\frac{1}{2}(|\beta|-|\alpha|+1)(2l-|\beta|-|\alpha|)}[1 - (-1)^{l-|\beta|}],$$
$$\text{when} \quad \alpha \subset \beta.$$

The basis we have been using suffers from a certain lack of symmetry in that the element m of $\{1, \cdots, m\}$ plays a preferred rôle. It is difficult to obtain a more symmetric basis so long as we deal with homology with integer coefficients. However, since the closed form integrated in (1.2) defines an element of a (de Rham) co-homology group with complex coefficients, we can obtain just as much information by considering homology with complex coefficients. Then, instead of the free Abelian group $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i)$ of rank 2^{m-1}, we have a 2^{m-1}-dimensional complex vector space $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i; \mathbf{C})$. Identifying the $\mathbf{e}_\beta$ with their images under the natural homomorphism of $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i)$ into $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i; \mathbf{C})$, we see that the $\mathbf{e}_\beta$ with $\beta \subset \{1, \cdots, m-1\}$ form a basis of the vector space $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i; \mathbf{C})$ and the linear relations (5.6) still hold. Similar relations may be obtained by choosing elements of $\{1, \cdots, m\}$ other than m to play the preferred rôle. By repeated application of these relations, we can express the $\mathbf{e}_\beta$ with $l - |\beta|$ odd as linear combinations with rational coefficients of the $\mathbf{e}_\beta$ with $l - |\beta|$ even. In fact, if $l - |\beta|$ is odd, we have

$$\mathbf{e}_\beta = \sum_{\substack{\gamma \supset \beta \\ l-|\gamma| \text{ even}}} c_{\frac{1}{2}(|\gamma|-|\beta|+1)}\mathbf{e}_\gamma, \tag{5.11}$$

where the coefficients c_r may be obtained by solving the recurrence relations

$$\sum_{r=1}^{n} (-1)^r \binom{2n}{2r-1} c_r = 1. \tag{5.12}$$

The first six coefficients are

$$c_1 = -\tfrac{1}{2}, \quad c_2 = -\tfrac{1}{4}, \quad c_3 = -\tfrac{1}{2},$$
$$c_4 = -\tfrac{17}{8}, \quad c_5 = -\tfrac{31}{2}, \quad c_6 = -\tfrac{691}{4}. \tag{5.13}$$

Thus the $\mathbf{e}_\beta$ with $l - |\beta|$ even constitute a symmetric basis of the vector space $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i; \mathbf{C})$.

Corresponding to the automorphism ψ_β of $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i)$, we have a non-singular linear transformation T_β of $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i; \mathbf{C})$ onto itself, which is still given formally by (2.2) and (2.3). In terms of the basis consisting of the $\mathbf{e}_\beta$ with $l - |\beta|$ even, T_β is represented by the non-singular $2^{m-1} \times 2^{m-1}$ matrix $M^{(\beta)}$ with rational elements, where

$$T_\beta(\mathbf{e}_\alpha) = \sum_{l-|\gamma| \text{ even}} M^{(\beta)}_{\gamma\alpha}\mathbf{e}_\gamma, \quad l - |\alpha| \text{ even}. \tag{5.14}$$

Using (2.2), (2.3), (4.18)–(4.21), and (5.11) we find that

$$M^{(\beta)}_{\gamma\alpha} = \delta_{\gamma\alpha} + N^{(\beta)}_{\gamma\alpha}, \tag{5.15}$$

where

$$N^{(\beta)}_{\gamma\alpha} = 0, \quad \text{unless} \quad \gamma = \beta \quad \text{and} \quad \alpha \subset \beta,$$
$$N^{(\beta)}_{\beta\alpha} = -(-1)^{\frac{1}{2}(|\beta|-|\alpha|)},$$
$$\text{when} \quad \alpha \subset \beta, \quad \alpha \neq \beta, \tag{5.16}$$
$$N^{(\beta)}_{\beta\beta} = -2, \quad \text{for} \quad l - |\beta| \text{ even},$$

and

$$N^{(\beta)}_{\gamma\alpha} = 0, \quad \text{unless} \quad \alpha \subset \beta \subset \gamma, \text{ when}$$
$$N^{(\beta)}_{\gamma\alpha} = (-1)^{\frac{1}{2}(|\beta|-|\alpha|-1)}c_{\frac{1}{2}(|\gamma|-|\beta|+1)}, \tag{5.17}$$
$$\text{for} \quad l - |\beta| \quad \text{odd}.$$

We now consider the cases $m = l + 1$ and $m = l + 2$. As the zero-dimensional compact homology group of a O-sphere (i.e., a pair of distinct points) is free Abelian of rank two, it follows from (5.1) that $H^c_l(\bar{\Sigma} - \bigcup_{i=1}^m \bar{\Sigma}_i)$ is a free Abelian group, of rank $2^{m-1} + 1$ in the case $m = l + 1$ and of rank $2^{m-1} + m - 2$ in the case $m = l + 2$. In both these cases, there exist β which satisfy both

$$\beta \subset \{1, \cdots, m-1\} \quad \text{and} \quad |\beta| = l.$$

For such β the O-chain e^β may be expressed as the difference of two O-simplices. Indeed, suppose $\beta = \{i_1, \cdots, i_l\}$, where the order of the elements is such that

$$\det(\pi_{i_1}, \cdots, \pi_{i_l}, \pi_\beta - \pi_{\beta m}) > 0.$$

Let e^β_+ and e^β_- be $(-1)^{l-1}$ times the O-simplices defined by the points

$$\mathbf{x}_0 = \pi_\beta, \qquad \mathbf{y} = (\pi_\beta^2 - 1)^{\frac{1}{2}} |\pi_\beta - \pi_{\beta m}|^{-1} (\pi_\beta - \pi_{\beta m})$$

and

$$\mathbf{x}_0 = \pi_\beta, \qquad \mathbf{y} = -(\pi_\beta^2 - 1)^{\frac{1}{2}} |\pi_\beta - \pi_{\beta m}|^{-1} (\pi_\beta - \pi_{\beta m}),$$

respectively. Then, with the given ordering for the elements of β, we have

$$e^{\beta} = e^{\beta}_{+} - e^{\beta}_{-}.$$

Hence,

$$\mathbf{e}_{\beta} = \mathbf{e}^{+}_{\beta} - \mathbf{e}^{-}_{\beta},$$

where

$$\mathbf{e}^{+}_{\beta} = \delta^{|\beta|}\, e^{\beta}_{+}, \qquad \mathbf{e}^{-}_{\beta} = \delta^{|\beta|}\, e^{\beta}_{-}.$$

A basis for $H^c_l(\Sigma - \bigcup_{i=1}^{m} \Sigma_i)$ in the cases $m = l + 1$ and $m = l + 2$ is provided by the $\mathbf{e}_{\beta}$ for

$$\beta \subset \{1, \cdots, m-1\}, \qquad |\beta| < l,$$

together with the $\mathbf{e}^{+}_{\beta}$ and $\mathbf{e}^{-}_{\beta}$ for $\beta \subset \{1, \cdots, m-1\}$, $|\beta| = l$. The dual basis of $H^c_l(\Sigma, \bigcup_{i=1}^{m} \Sigma_i)$ is now given by

$$\begin{aligned}
&{}^{\beta}e = (-1)^{\frac{1}{2}(l-|\beta|)(l-|\beta|-1)}(e_{\beta} - e_{\beta m}),\\
&\qquad \text{for} \quad \beta \subset \{1, \cdots, m-1\}, \quad 0 < |\beta| < l,\\
&{}^{\varnothing}e = (-1)^{\frac{1}{2}l(l+1)} e_m, \qquad (5.18)\\
&{}^{\beta}_{+}e = \sum_{\gamma \subset \beta} (-1)^{l-|\gamma|} e_{\gamma m}, \quad {}^{\beta}_{-}e = e_{\beta m} - e_{\beta},\\
&\qquad \text{for} \quad \beta \subset \{1, \cdots, m-1\}, \quad |\beta| = l
\end{aligned}$$

as one easily verifies with the aid of (4.18), (4.19), (4.20), (4.21), and the relations

$$\begin{aligned}
\mathrm{KI}\,[\mathbf{e}^{+}_{\beta}, e_{\beta}] = \mathrm{KI}\,[e^{\beta}_{+}, e^{\beta}] &= 1,\\
\mathrm{KI}\,[\mathbf{e}^{-}_{\beta}, e_{\beta}] = \mathrm{KI}\,[e^{\beta}_{-}, e^{\beta}] &= -1,\\
\mathrm{KI}\,[\mathbf{e}^{+}_{\beta}, e_{\beta m}] &= 1,\\
\mathrm{KI}\,[\mathbf{e}^{-}_{\beta}, e_{\beta m}] &= 0,
\end{aligned}$$

holding for $\beta \subset \{1, \cdots, m-1\}$, $|\beta| = l$. On writing $\mathbf{e}_{\gamma m}$ for $\gamma \subset \{1, \cdots, m-1\}$, $|\gamma| < l$ as a linear combination of the $\mathbf{e}_{\beta}$ with $\beta \subset \{1, \cdots, m-1\}$, $|\beta| < l$ and the $\mathbf{e}^{+}_{\beta}$ and $\mathbf{e}^{-}_{\beta}$ with $\beta \subset \{1, \cdots, m-1\}$, $|\beta| = l$, and evaluating the coefficients as before, we find that (5.6) is still valid in the cases $m = l + 1$ and $m = l + 2$. It follows that the linear relations (5.11) also remain valid. So too do the matrix representations given by (5.8)–(5.10) and (5.15)–(5.17), respectively, though they now refer only to the subgroup (subspace) of $H^c_l(\Sigma - \bigcup_{i=1}^{m} \Sigma_i)$ $[H^c_l(\Sigma - \bigcup_{i=1}^{m} \Sigma_i; \mathbf{C})]$ generated (spanned) by the $\mathbf{e}_{\beta}$, which is mapped onto itself by each of the $\psi_{\beta}(T_{\beta})$. However, as the homology class of the original cycle of integration $\bar{\Gamma} = (-1)^{l}\mathbf{e}_{\varnothing}$ belongs to this subgroup (subspace), these matrix representations still contain enough information to enable us to find the value of $J(P)$ on any Riemann sheet that can be reached by a succession of loops α_{β}.

It is interesting to note that, when l is odd, (5.6) with $\gamma = \varnothing$ expresses $2\bar{\Gamma}$ as a linear combination of $\mathbf{e}_{\beta}$ with β in B. Hence, the original integral $J(P)$ may be written as a linear combination of its discontinuity functions (2.4). Unfortunately, this does not work in the physically interesting cases of $l = 4$ and $l = 2$.

Variation of Green's Functions

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The variation of the Green's function of a linear differential operator is computed as the variation of an n-tuple integral with variable boundary. This generalization of Hadamard formula is shown to lead naturally to the method of "invariant imbedding" of R. Bellman. Three applications of the general formalism are given: the Dirichlet problem, the neutron or photon transport in a plane parallel anisotropically scattering slab, and scattering in a central field where three identities used in potential scattering are shown to be a consequence of the invariance of the asymptotic Green's function.

I. INTRODUCTION

IDENTITIES analogous to Green's identities are common in mathematical physics mainly through the variational principles. Among notable examples, we mention an identity used by K. M. Case[1] in neutron-transport theory, and the Kato identity[2,3] (with all its variants) in scattering theory. From these identities, it is possible to derive remarkable functional relations, generally under the form of nonlinear integro-differential equations, some of which have already been put to use in radiative transfer theory.[4]

The purpose of this paper is twofold: we first compute a general expression for the variation of the Green's function of a linear differential operator to obtain a generalization of the Hadamard formula of some importance in applied functional analysis.[5,15] We next show how the method of "invariant imbedding" of Bellman, Kalaba, and Wing[6] (which is used recently in radiative transfer theory, neutron transport theory,[6] electron backscattering theory,[7] and potential scattering[8]) is derived as a particular case of the Hadamard formula. From invariance principles, a set of two functional equations satisfied by Green's function is obtained. These equations are related to the Ambarzumian–Chandrasekhar invariance principles of radiative transfer theory. For further examples of the Hadamard formula, we show its relation to Kato identity; we also show how the variation of the Green's function can lead to a neat and unified treatment of some fundamental identities of scattering theory by a central field, like a recent generalization of the virial theorem by Robinson and Hirschfelder.[9]

II. THE GENERALIZED HADAMARD FORMULA

Let F be a linear differential operator, U a function of the N independent variables, $x^1, \cdots, x^N$, satisfying the linear partial differential equation

$$FU - Q_u = 0, \tag{1}$$

where Q_u is a given function. We define the adjoint operator G through the identity

$$VFU - UGV = \operatorname{div} \mathbf{J}(v, V), \tag{2}$$

where the components of vector $\mathbf{J}$ are bilinear forms of U, V, and their derivatives. We will not delve into details of the well-known computation of $\mathbf{J}$.[10]

Let

$$\mathfrak{L}_0 = \tfrac{1}{2}(VFU - UGV), \tag{3}$$

$$\mathfrak{L} = \mathfrak{L}_0 - VQ_u - UQ_v, \tag{4}$$

where Q_v is also a given function.

If $\mathfrak{L}$ is taken as Lagrangian, the Euler–Lagrange equations are

$$\delta\mathfrak{L}/\delta V = FU - Q_u = 0, \tag{5}$$

$$\delta\mathfrak{L}/\delta U = GV - Q_v = 0. \tag{6}$$

To this set of equations, we must add boundary conditions. (We assume from now on that boundary conditions are adjoint of each other.) If we add to F a linear integral operator whose kernel is self-adjoint, we do not modify the expression of J (Eq. 2). Let us compute the variation of the N-tuple integral with variable boundary[11]

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$$I = \int_N \mathfrak{L}\, dv, \qquad dv = dx^1 \cdots dx^N. \tag{7}$$

Define the dummy variable τ as the independent variable and

$$\begin{aligned} \delta U &\equiv X^u(U, V, x^i, \tau)\, \delta\tau, \\ \delta V &\equiv X^v(U, V, x^i, \tau)\, \delta\tau, \\ \delta x^i &= X^i(U, V, x^i, \tau)\, \delta\tau. \end{aligned} \tag{8}$$

Then

$$\frac{\delta I}{\delta\tau} = \int_N D\mathfrak{L}\, dv + \oint_{N-1} (\mathfrak{L}X^n + D^n\mathfrak{L})\, dS \tag{9}$$

with

$$D\mathfrak{L} \equiv \frac{\partial \mathfrak{L}}{\partial \tau} + \frac{\delta \mathfrak{L}}{\delta U}\frac{\partial U}{\partial \tau} + \frac{\delta \mathfrak{L}}{\delta V}\frac{\partial V}{\partial \tau}, \tag{10}$$

and X^n, D^n the components normal to the surface of vectors whose Cartesian components are, respectively, X^k and

$$\begin{aligned} D^k\mathfrak{L} \equiv \frac{\delta \mathfrak{L}}{\delta U_{,k}}\frac{\partial U}{\partial \tau} + \frac{\delta \mathfrak{L}}{\delta V_{,k}}\frac{\partial V}{\partial \tau} + \frac{\delta \mathfrak{L}}{\delta U_{,ki}}\frac{d}{dx^i}\left(\frac{\partial U}{\partial \tau}\right) \\ + \frac{\delta \mathfrak{L}}{\delta V_{,ki}}\frac{d}{dx^i}\left(\frac{\partial V}{\partial \tau}\right) + \cdots \end{aligned} \tag{11}$$

with $U_{,k} = \partial U/\partial x^k$, etc. Moreover,

$$\begin{aligned} \delta U/\delta\tau &\equiv X^u = \partial U/\partial\tau + U_{,i}X^i, \\ \delta V/\delta\tau &\equiv X^v = \partial V/\partial\tau + V_{,i}X^i. \end{aligned} \tag{12}$$

We assume that the Euler–Lagrange equations [(5) and (6)] are satisfied. Then,

$$I = -\tfrac{1}{2}(V, Q_u) - \tfrac{1}{2}(U, Q_v).$$

The independent sources Q_u and Q_v are specialized to

$$Q_u = \prod_1^N \delta(x^i - x_0^i), \qquad Q_v = \prod_1^N \delta(x^i - x_1^i)$$

with

$$\int_{-\infty}^{\infty} \delta(x^i - x_0^i)\, dx^i = 1;$$

and

$$\begin{aligned} U &\equiv U(\mathbf{r}_1 \mid \mathbf{r}_0), \qquad V \equiv V(\mathbf{r}_1 \mid \mathbf{r}_0), \\ \mathbf{r}_0 &= (x_0^i), \qquad \mathbf{r}_1 = (x_1^i) \end{aligned}$$

are, respectively, the Green's function of the direct and adjoint problem.[12]

From the reciprocity theorem, we have

$$V(\mathbf{r} \mid \mathbf{r}_1) = U(\mathbf{r}_1 \mid \mathbf{r}) \tag{13}$$

[12] Unless explicitly stated, sources are not on the surface.

and therefore,

$$I = -U(\mathbf{r}_1 \mid \mathbf{r}_0). \tag{14}$$

We have also

$$\begin{aligned} \int_N D\mathfrak{L}\, dv &= \int_N \frac{\partial \mathfrak{L}}{\partial \tau}\, dv \\ &= \int_N \frac{\partial \mathfrak{L}_0}{\partial \tau}\, dv - \int_N \frac{\partial}{\partial \tau}[VQ_u + UQ_v]\, dv \\ &= \frac{1}{2}\int_N V\frac{\partial F}{\partial \tau}\, U\, dv + \frac{1}{2}\int_N U\frac{\partial G}{\partial \tau}\, V\, dv \\ &\quad - \int_N V\frac{\partial Q_u}{\partial \tau}\, dv - \int_N U\frac{\partial Q_v}{\partial \tau}\, dv. \end{aligned}$$

Using the formal properties of the derivative of Dirac's function,

$$\begin{aligned} &\int_N V\frac{\partial Q_u}{\partial \tau}\, dv + \int_N U\frac{\partial Q_v}{\partial \tau}\, dv \\ &= \int_N \left[V(\mathbf{r} \mid \mathbf{r}_1)\, \delta^{(1)}(\mathbf{r} - \mathbf{r}_0(\tau))\frac{\partial \mathbf{r}_0}{\partial \tau} \right. \\ &\quad \left. + U(\mathbf{r} \mid \mathbf{r}_0)\, \delta^{(1)}(\mathbf{r} - \mathbf{r}_1(\tau))\frac{\partial \mathbf{r}_1}{\partial \tau} \right] dv \\ &= \frac{\partial \mathbf{r}_0}{\partial \tau}\operatorname{grad}_0 U(\mathbf{r}_1 \mid \mathbf{r}_0) + \frac{\partial \mathbf{r}_1}{\partial \tau}\operatorname{grad}_1 U(\mathbf{r}_1 \mid \mathbf{r}_0). \end{aligned} \tag{15}$$

Define

$$\int_N \mathfrak{D}_\tau \mathfrak{L}_0\, dv \equiv \int_N U\frac{\partial G}{\partial \tau}\, V\, dv + \int_N V\frac{\partial F}{\partial \tau}\, U\, dv. \tag{16}$$

From (9), (14), (15), and (16)

$$\begin{aligned} \frac{\delta U(\mathbf{r}_1 \mid \mathbf{r}_0)}{\delta \tau} &= \left[\sum_i X_0^i \frac{\partial U}{\partial x_0^i} + \sum_i X_1^i \frac{\partial U}{\partial x_1^i} \right] \\ &\quad - \left[\int_N \mathfrak{D}_\tau \mathfrak{L}_0\, dv + \oint_{N-1} (\mathfrak{L}X^n + D^n\mathfrak{L})\, dS \right], \end{aligned} \tag{16a}$$

which is the first form of our result. The variation of the Green's function is the sum of two terms: the first bracket of (16a) is the variation of the Green's function when points $\mathbf{r}_1$, $\mathbf{r}_0$ are displaced, and the second bracket illustrates the fact that $U(\mathbf{r}_1 \mid \mathbf{r}_0)$ is a functional and therefore reflects any displacement of the boundary or change of the substratum. Introducing (11) into (16a), we obtain a second (and sometimes more useful) form:

$$\begin{aligned} \frac{\delta U(\mathbf{r}_1 \mid \mathbf{r}_0)}{\delta \tau} &= \left[\sum_i \left(X_0^i \frac{\partial U}{\partial x_0^i} + X_1^i \frac{\partial U}{\partial x_1^i} \right) - \oint_{N-1} \mathfrak{C}^n\, dS \right] \\ &\quad - \left[\int_N \mathfrak{D}_\tau \mathfrak{L}_0\, dv + \oint_{N-1} R^n\, dS \right], \end{aligned} \tag{16b}$$

$$\mathfrak{A}^i \equiv \sum_j \mathfrak{I}^i_j X^j + \sum_{j,l} S^{jl}_i X^j_{,l},$$

$$\mathfrak{I}^i_j \equiv \Big(\mathfrak{L}\delta^i_j - \frac{\delta\mathfrak{L}}{\delta U_{,i}} U_{,j} - \frac{\delta\mathfrak{L}}{\delta V_{,i}} V_{,j} - \frac{\delta\mathfrak{L}}{\delta U_{,il}} U_{,jl} - \frac{\delta\mathfrak{L}}{\delta V_{,il}} V_{,jl} \cdots\Big), \quad (17)$$

$$S^{jl}_i \equiv -\frac{\delta\mathfrak{L}}{\delta U_{,il}} U_{,j} - \cdots,$$

$$\mathfrak{R}^i \equiv \frac{\delta\mathfrak{L}}{\delta U_{,i}} X^u + \frac{\delta\mathfrak{L}}{\delta V_{,i}} X^v + \frac{\delta\mathfrak{L}}{\delta U_{,ij}} X^u_{,j} + \frac{\delta\mathfrak{L}}{\delta V_{,ij}} X^v_{,j} + \cdots. \quad (18)$$

We have written derivatives up to the second order only. Either form (16a) or form (16b) can be used. For instance, in neutron transport theory, boundary conditions impose $R^u = 0$, and form (16b) is more appropriate. On the other hand, when τ is not explicit, $\mathfrak{D}_\tau\mathfrak{L} = 0$ and $D^u\mathfrak{L} = 0$, and form (16a) is more appropriate.

We must ask under what conditions $\delta U(\mathbf{r}_1 \mid \mathbf{r}_0)/\delta\tau$ equals to zero. For instance, let us assume that boundary conditions have an intrinsic character. That is, the boundary conditions, and therefore also the Green's function, are invariant for Euclidian displacements, i.e., for translations and rotations. Let $X^i_0 = X^i_1 = \Omega^i$, where Ω^i is the cosine director of unit vector $\boldsymbol{\Omega}$. Translation invariance yields

$$\boldsymbol{\Omega}\,\mathrm{grad}_1\, U(\mathbf{r}_1 \mid \mathbf{r}_0) + \boldsymbol{\Omega}\,\mathrm{grad}_0\, U(\mathbf{r}_1 \mid \mathbf{r}_0) - \oint \sum_j \mathfrak{I}^u_j \Omega^j\, dS = 0. \quad (19)$$

This equation is verified for any $\boldsymbol{\Omega}$ and therefore

$$\mathrm{grad}_1\, U(\mathbf{r}_1 \mid \mathbf{r}_0) + \mathrm{grad}_0\, U(\mathbf{r}_1 \mid \mathbf{r}_0) - \oint \mathfrak{I}^u\, dS = 0, \quad (20)$$

where $\mathfrak{I}^u$ is the vector whose components are $\mathfrak{I}^u_j$. Similarly, rotational invariance yields

$$\mathbf{r}_1 \times \mathrm{grad}_1\, U(\mathbf{r}_1 \mid \mathbf{r}_0) + \mathbf{r}_0 \times \mathrm{grad}_0\, U(\mathbf{r}_1 \mid \mathbf{r}_0) - \oint (\mathbf{r} \times \mathfrak{I}^u)\, dS = 0. \quad (21)$$

III. AN IDENTITY

We now show the close connection between an identity (used time and again in various forms) and the variational formulas (16a) and (16b). Let us consider a one parameter (τ) family of problems. A subscript will label the problem in the family. Let U_β and V_α be, respectively, solutions of

$$F_\beta U_\beta - Q^u_\beta = 0, \qquad G_\alpha V_\alpha - Q^v_\alpha = 0, \quad (22)$$

where α, β are given values of the parameter and Q^u_β, Q^v_α given functions not necessarily equal to Dirac's functions. U_α and V_α satisfy adjoint boundary conditions on the surface. Both the boundary conditions and the surface are assumed to be independent of the parameter. We have the identity

$$K_{\alpha\beta} \equiv (V_\alpha, F_\beta U_\beta) - (V_\alpha, Q^u_\beta) - (U_\beta, G_\alpha V_\alpha) + (U_\beta, Q^v_\alpha) = 0. \quad (23)$$

We define

$$\delta U_\alpha \equiv U_\beta - U_\alpha, \qquad \delta V_\alpha \equiv V_\beta - V_\alpha,$$
$$\delta F_\alpha \equiv F_\beta - F_\alpha, \qquad \delta G_\alpha \equiv G_\beta - G_\alpha.$$

Let $\beta \to \alpha$, and, keeping only first-order terms,

$$K_{\alpha\beta} = \tfrac{1}{2}(V_\alpha, \delta F_\alpha\, U_\alpha) + \tfrac{1}{2}(U_\alpha, \delta G_\alpha\, V_\alpha) - (V_\alpha, Q^u_\beta) + (U_\beta, Q^v_\beta) + \frac{1}{2}\int_N \mathrm{div}\,[\mathcal{J}(U_\alpha, \delta V_\alpha) + \mathcal{J}(V_\alpha, \delta U_\alpha)]\, dv = 0. \quad (24)$$

The surface integral vanishes and we have the first-order relation

$$(V_\alpha, Q^u_\beta) - (U_\beta, Q^v_\alpha) = \tfrac{1}{2}(U_\alpha, \delta G_\alpha\, V_\alpha) + \tfrac{1}{2}(V_\alpha, \delta F_\alpha\, U_\alpha). \quad (25)$$

Let $Q^u_\beta = \delta(\mathbf{r} - \mathbf{r}^\beta_0)$, $Q^v_\alpha = \delta(\mathbf{r} - \mathbf{r}^\alpha_1)$, $\mathbf{r}^\alpha_1 \neq \mathbf{r}^\alpha_0$. If we let $\alpha = \beta$, we have the reciprocity theorem

$$V_\alpha(\mathbf{r}_0 \mid \mathbf{r}_1) = U_\alpha(\mathbf{r}_1 \mid \mathbf{r}_0), \quad (26)$$

where $V_\alpha(\mathbf{r} \mid \mathbf{r}_1)$ and $U_\beta(\mathbf{r} \mid \mathbf{r}_0)$ are solutions of (22). Introducing (26) in (25), we have

$$\tfrac{1}{2}(V_\alpha, \delta F_\alpha\, U_\alpha) + \tfrac{1}{2}(U_\alpha, \delta G_\alpha\, V_\alpha) = -\delta U_\alpha(\mathbf{r}_1 \mid \mathbf{r}_0) \quad (27)$$

or

$$\frac{\delta U(\mathbf{r}_1 \mid \mathbf{r}_0)}{\delta\tau} = -\int_N \mathfrak{D}_\tau\mathfrak{L}_0\, dv$$

in the notation of Sec II as a special case of (16a). Identity (23) with $\alpha = \beta$ has been used by Case[1] to derive various forms of the reciprocity principle. When $\alpha \neq \beta$, identity (23) has close connections with the Kato identity,[2,3] and $F \equiv H - E$ with H the Hamiltonian and E the energy. However, as we shall see in Sec. IV C, surface and sources are removed to infinity.

IV. APPLICATIONS

A. The Dirichlet Problem

We have

$$\mathfrak{L}_0 = \tfrac{1}{2}(U\Delta V + V\Delta U). \tag{28}$$

There is no explicit dependence on τ and $\mathfrak{D}_\tau\mathfrak{L}_0 = 0$. The homogeneous Dirichlet boundary condition is $U(\mathbf{r} \mid \mathbf{r}_0) = 0$ and $V(\mathbf{r} \mid \mathbf{r}_1) = 0$ for $\mathbf{r}$ on the surface. Therefore, $X^U = X^V = X^*_{,n} = X^*_{,n} = 0$ and $R^n = 0$. If self-adjointness is taken into account, and if $\mathbf{r}_1$ and $\mathbf{r}_0$ are not on the boundary, Eq. (16b) yields

$$\frac{\delta U(\mathbf{r}_1 \mid \mathbf{r}_0)}{\delta\tau} = \frac{\delta\mathbf{r}_1}{\delta\tau}\,\mathrm{grad}_1\, U(\mathbf{r}_1 \mid \mathbf{r}_0) + \frac{\delta\mathbf{r}_0}{\delta\tau}\,\mathrm{grad}_0\, U(\mathbf{r}_1 \mid \mathbf{r}_0) - \oint \frac{\delta n}{\delta\tau}\frac{\partial U(\mathbf{r}_1 \mid \mathbf{r})}{\partial n}\frac{\partial U(\mathbf{r} \mid \mathbf{r}_0)}{\partial n}\,dS, \tag{29}$$

where $\delta n = X^n\delta\tau$ is the normal displacement. Usually, the Green's function is defined as the solution of $\Delta U(\mathbf{r} \mid \mathbf{r}_0) = 4\pi\delta(\mathbf{r} - \mathbf{r}_0)$. If $\mathbf{r}_0$ and $\mathbf{r}_1$ are fixed, we obtain the classical Hadamard formula[5]

$$\delta U(\mathbf{r}_1 \mid \mathbf{r}_0) = -\frac{1}{4\pi}\oint \frac{\partial U(\mathbf{r}_1 \mid \mathbf{r})}{\partial n}\frac{\partial U(\mathbf{r} \mid \mathbf{r}_0)}{\partial n}\,\delta n\,dS. \tag{30}$$

B. Neutron and Photon Transport

The method of "invariant imbedding" of Bellman, Kalaba, and Wing[6] is, in fact, contained in formula (16b). The problem, set up initially by Bellman, was to search for functional relations between particular Green's functions: the reflexion and transmission function of slab-like media. The problem was later generalized to stratifiable inhomogeneous media with isotropic scattering. However, we can further generalize the results of Bellman *et al.* to arbitrary Green's functions (although the problem is simpler), to arbitrary media (i.e., not necessarily monotone under inclusion), and to anisotropic scattering. The variational method used here has the advantage over the "invariant imbedding" methods in that no "particle counting" is necessary. It should be remembered that "invariant imbedding" was motivated by the conversion of two-point boundary-value problems into initial-value problems. Although equations are nonlinear, the switch from Fredholm-like equations to Volterra-like equations has many computational advantages.

Since this application is intended to illustrate the flexibility of the variational expression for the Green's function, we shall restrict our illustration to the time-independent case of the plane-parallel, anisotropically scattering, atmosphere of finite optical thickness a.

Let $\phi(x, \mu)$ be the intensity of radiation in the direction $+\mu$ ($0 < \mu = \cos\theta \leq 1$), where θ is the angle in the direction of the entering normal (i.e., along the positive axis). Let $x = 0$ be the left boundary and $x = a$ be the right boundary. The Boltzmann equation takes the form

$$\mu\frac{d\phi(x, \mu)}{dx} + \phi(x, \mu) = c(x)\int_{-1}^{1}\phi(x, \mu')f(\mu' \to \mu)\,d\mu' + S(x, \mu), \tag{31}$$

where $c(x)$ is the mean number of secondaries scattered for one primary particle (either photon or neutron), $S(x, \mu)$ the source intensity, and $f(\mu' \to \mu)$ the probability that a particle moving in direction μ' is thrown into the direction μ after scattering. We have the normalization

$$\int_{-1}^{1} f(\mu' \to \mu)\,d\mu' = \int_{-1}^{1} f(\mu' \to \mu)\,d\mu = 1.$$

Moreover, time-reflection symmetry gives

$$f(\mu' \to \mu) = f(-\mu \to -\mu')$$

and spatial-reflection symmetry gives $f(\mu' \to \mu) = f(\mu \to \mu')$. There are no internal sources, but since the slab is irradiated by a plane-parallel source, we have the following boundary conditions:

$$\phi(0, \mu) = 0, \qquad \mu > 0 \tag{32}$$
$$\phi(a, \mu) = \delta(\mu - \mu_0), \qquad \mu, \mu_0 < 0.$$

In order to apply Eq. (16b), we must convert these boundary conditions into surface sources, otherwise no Green's function can be defined. Let us take $S(x, \mu) = Q\delta(x - a)\delta(\mu - \mu_0)$. Integrating (31) from $a - \epsilon$ to $a + \epsilon$,

$$\mu[\phi(a + \epsilon, \mu) - \phi(a - \epsilon, \mu)] = Q\,\delta(\mu - \mu_0). \tag{33}$$

Since $\phi(a + \epsilon) = 0$ and

$$\lim_{\epsilon \to 0}\phi(a - \epsilon, \mu) = \delta(\mu - \mu_0), \quad Q = -\mu_0 = +|\mu_0|. \tag{34}$$

The adjoint flux is $\phi^*(x, \mu)$, the solution of

$$-\mu\frac{d\phi^*(x, \mu)}{dx} + \phi^*(x, \mu) = c(x)\int_{-1}^{1}\phi^*(x, \mu')f(\mu \to \mu')\,d\mu' + S^*(x, \mu). \tag{35}$$

Intensity $\phi(x, \mu)$ can be rewritten as the Green's function $G(x, \mu \mid a, \mu_0)$. We choose $S^*(x, \mu) =$

$-\mu_1\delta(\mu - \mu_1)$ with $\mu_1 < 0$ and with $\phi^*(x, \mu) \equiv G^*(x, \mu \mid a_1, + \mu_1)$. It is easy to check

$$G^*(x, \mu \mid a, \mu_1) = G(x, -\mu \mid a, -\mu_1) \tag{36a}$$

and

$$|\mu|\, G(x, \mu \mid a, \mu_1) = |\mu_1|\, G(a, -\mu_1 \mid x, -\mu) \tag{36b}$$

(the reciprocity principle).

The volume V in the space $x \times \mu$ is topologically equivalent to the lateral surface of a right cylinder of length a. The boundary is the sum of the two edges of the finite cylinder, and reduces to the boundary of the x subspace.

From the definition of I:

$$\begin{aligned} I &= \frac{|\mu_1|}{2} \int_2 G(x, \mu \mid a, \mu_0)\, \delta(x - \lambda)\, \delta(\mu - \mu_1)\, dx\, d\mu \\ &\quad + \frac{|\mu_0|}{2} \int_2 G^*(x, \mu \mid a, \mu_1)\, \delta(x - \lambda)\, \delta(\mu - \mu_0)\, dx\, d\mu \\ &= \frac{|\mu_1|}{2} G(a, \mu_1 \mid a, \mu_0) + \frac{|\mu_0|}{2} G^*(a, \mu_0 \mid a, \mu_1) \\ &= \frac{|\mu_1|}{2} G(a, \mu_1 \mid a, \mu_0) + \tfrac{1}{2}\, |\mu_0|\, G(a, -\mu_0 \mid a, -\mu_1) \\ &= |\mu_1|\, G(a, \mu_1 \mid a, \mu_0). \end{aligned} \tag{37}$$

We separate the scattered from the unscattered flux and write

$$G(a, \mu \mid a, \mu_0) = \delta(\mu - \mu_0) + S(\mu, \mu_0)/|\mu|, \tag{38}$$

where $S(\mu, \mu_0) = 0$ for $\mu < 0$. The number of reflected particles in direction $\mu > 0$ for a collimated plane source $|\mu_0|\, \delta(x - a)\delta(\mu - \mu_0)$ is $S(\mu, \mu_0)$. The following relations are the immediate consequences of (38) and (36)

$$\begin{aligned} S(\mu, \mu_0) &= S(-\mu_0, -\mu), \\ S^*(\mu, \mu_0) &= S(-\mu, -\mu_0). \end{aligned} \tag{39}$$

We imbed the problem in a family of problems with variable thickness a and therefore $a \equiv \tau$, the variational parameter. The boundary conditions are unchanged[13] and $R^n = 0$. Moreover, $X^n = dx/d\tau$ on the surface 1 at $x = \lambda$ and $X^n = 0$ on surface 2 at $x = 0$. Using Eqs. (17) and (31), the surface integral $\oint_1 \mathfrak{A}^n\, dS$ reads

$$\begin{aligned} \oint_1 \mathfrak{A}^n\, dS &= \int_{-1}^{1} G(a, \mu \mid a, \mu_0)\, d\mu \\ &\quad \times \int_{-1}^{1} [\delta(\mu - \mu') - c(a) f(\mu' \to \mu)] \\ &\quad \times G(a, -\mu' \mid a, -\mu_1)\, d\mu'. \end{aligned} \tag{40}$$

In order to avoid the complication of surface sources in (16b), we remove them infinitesimally at thickness $a - \epsilon$. To order ϵ, we have

$$\frac{\delta S(\mu_1, \mu_0)}{\partial \tau} = -\oint_1 \mathfrak{A}^n\, dS. \tag{41}$$

Since $\mu_1 < 0$ and $\mathfrak{D}_\tau \mathfrak{L}_0 = 0$, $c(x)$ being an explicit function of position but not of thickness a.

Introducing (38) into (40) and (41),

$$\begin{aligned} -\frac{\delta S(\mu_1, \mu_0)}{\delta \tau} &= \int_{-1}^{1} d\mu \left[\delta(\mu - \mu_0) + \frac{S(\mu, \mu_0)}{|\mu|}\right] \\ &\quad \times \int_{-1}^{1} \left[\delta(\mu - \mu') - c(a) f(\mu' \to \mu)\right]\left[\delta(\mu' - \mu_1) + \frac{S(-\mu', -\mu_1)}{|\mu'|}\right] d\mu' \\ &= \delta(\mu_0 - \mu_1) + \frac{S(-\mu_0, -\mu_1)}{|\mu_0|} + \frac{S(\mu_1, \mu_0)}{|\mu_1|} - c(a) f(\mu_1 \to \mu_0) \\ &\quad - c(a) \int_{-1}^{1} S(-\mu', -\mu_1) f(\mu' \to \mu_0) \frac{d\mu'}{|\mu'|} - c(a) \int_{-1}^{1} \frac{S(\mu, \mu_0)}{|\mu|} f(\mu_1 \to \mu)\, d\mu \\ &\quad - c(a) \int_{-1}^{1} \int_{-1}^{1} \frac{S(\mu, \mu_0)}{|\mu|} f(\mu' \to \mu) \frac{S(-\mu', -\mu_1)}{|\mu'|}\, d\mu\, d\mu' + \int_{-1}^{1} \frac{S(\mu, \mu_0) S(-\mu, -\mu_1)}{\mu^2}\, d\mu. \end{aligned} \tag{42}$$

From (39), since $\mu_0\mu_1 < 0$, $\delta(\mu_1 - \mu_0) = 0$, and $S(\mu, \mu_0)S(-\mu, -\mu_1) = 0$, we have

$$\begin{aligned} -\frac{\delta S(\mu_1, \mu_0)}{\delta a} &= S(\mu_1, \mu_0)\left(\frac{1}{|\mu_1|} + \frac{1}{|\mu_0|}\right) - c(a)\Big[f(\mu_0 \to \mu_1) + \int_{-1}^{1} f(\mu_1 \to \mu) \frac{S(\mu, \mu_0)}{|\mu|}\, d\mu \\ &\quad + \int_{-1}^{1} f(\mu_0 \to \mu) \frac{S(\mu_1, \mu)}{|\mu|}\, d\mu + \int_{-1}^{1} \int_{-1}^{1} \frac{S(\mu, \mu_0)}{|\mu|} f(\mu \to \mu') \frac{S(\mu_1 \to \mu')}{|\mu'|}\, d\mu\, d\mu'\Big]. \end{aligned} \tag{43}$$

[13] When the surface sources are arbitrary or when the surface has curvature, the problem is more complicated and lies outside the scope of this paper.

Since $S(\mu_1, \mu_0)$ is also an explicit function of a and μ_1, μ_0 are independent of a[13] $\delta S/\delta a = \partial S/\partial a$ Eq. (43) is the final result, a generalization to anisotropic scattering of a result derived by Ueno,[4] Bellman and Kalaba[6] by different methods. An alternate derivation is the invariance equation (20), since the Green's function is invariant for a displacement of the origin. We have

$$\frac{\partial}{\partial \tau} = \frac{\partial x_0}{\partial \tau}\frac{\partial}{\partial x_0} + \frac{\partial x_1}{\partial \tau}\frac{\partial}{\partial x_1} + \frac{\partial a}{\partial \tau}\frac{\partial}{\partial a},$$

while S is not an explicit function of x_0 and x_1. Therefore, $\delta S(\mu_1, \mu_0)/\delta \tau = 0$ gives

$$(\partial/\partial x_0 + \partial/\partial x_1)S(\mu_1, \mu_0) = -(\partial/\partial a)S(\mu_1, \mu_0)$$

and the invariance equation reads

$$(\partial/\partial a)S(\mu_1, \mu_0) + \oint \mathbf{n}\mathfrak{J}^n \, dS = 0 \qquad (44)$$

with the normal pointing along x. Equation (44) is identical with (41).

C. Scattering by a Central Field

The variation of the Green's function can provide a neat and unified treatment of some fundamental identities of scattering theory.[3]

We define the reduced Hamiltonian

$$\mathbf{H} \equiv (2m/\hbar^2)H, \qquad \mathbf{V}(r) \equiv (2m/\hbar^2)V(r), \qquad (45)$$

and

$$\mathbf{H} = -\Delta + \mathbf{V}.$$

Operator $\mathbf{F}$ is

$$\mathbf{F} = \mathbf{H} - k^2. \qquad (46)$$

The Green's function will be defined for a point source removed to infinity in the direction of $-\mathbf{k}_i$

$$\lim_{r_0 \to \infty} U(\mathbf{r}_1 \mid \mathbf{r}_0) = \exp i\mathbf{k}_i\mathbf{r}_1 + F(\theta)\,[(\exp i\mathbf{k}_f\mathbf{r}_1)/r_1] \equiv \psi_i. \qquad (47)$$

With $|\mathbf{k}_i| = |\mathbf{k}_f| = k$ and $\pi - \theta$ the angle between k_0 and k_1, we have

$$\lim_{a \to \infty} U(\mathbf{r}_1 \to \mathbf{k}_f a \mid \mathbf{r}_0 \to -\mathbf{k}_i a) = \lim_{r_1 \to \infty} \exp i\mathbf{k}_i\mathbf{r}_1 \equiv U_\infty(\mathbf{r}_1 \mid \mathbf{r}_0). \qquad (48)$$

At large distance, the uncollided flux dominates, and we can state that $U_\infty(\mathbf{r}_1 \mid \mathbf{r}_0)$ is invariant for any transformation which leaves $\mathbf{k}_f\mathbf{r}_1$ and $\mathbf{k}_i\mathbf{r}_0$ invariant. Since k and $\mathbf{r}_1$, $\mathbf{r}_0$ occur only in the products $\mathbf{k}_i\mathbf{r}_0$ and $\mathbf{k}_f\mathbf{r}_1$, we can assume $U_\infty(\mathbf{r}_1 \mid \mathbf{r}_0)$ to be a member of a two-parameter family of functions:

$$U_\infty(\mathbf{r}_1 \mid \mathbf{r}_0) \equiv G(\lambda\mathbf{r}_1, \lambda\mathbf{r}_0 \mid k/\lambda, p\mu)|_{\lambda=\mu=1}, \qquad (49)$$

where λ and μ are independent variables, and p is any parameter of $\mathbf{H}$, except the parameter of k. Therefore,

$$\delta U_\infty(\mathbf{r}_1 \mid \mathbf{r}_0)/\delta\lambda|_{\lambda=\mu=1} = 0 \quad \text{and} \quad \delta U_\infty(\mathbf{r}_1 \mid \mathbf{r}_0)/\delta\mu|_{\lambda=\mu=1} = 0. \qquad (50)$$

The last equation is a consequence of the fact that $U_\infty(\mathbf{r}_1|\mathbf{r}_0)$ is independent of any other parameter except k. Using identity (16a) and

$$\frac{\delta U_\infty(\mathbf{r}_1 \mid \mathbf{r}_0)}{\delta\tau} = -\lim_{a\to\infty}\int \mathfrak{D}_\tau \mathfrak{L}_0 \, dv - \lim_{a\to\infty}\oint D^n\mathfrak{L}\, dS = \lim_{a\to\infty}\frac{\delta U(\mathbf{r}_1 \mid \mathbf{r}_0)}{\delta\tau} \qquad (51)$$

(since $X^k = X_1^i = X = 0$), therefore,

$$\lim_{a\to\infty}\int \mathfrak{D}_\lambda\mathfrak{L}_0\, dv|_{\lambda=\mu=1} = -\lim_{a\to\infty}\oint D^n\mathfrak{L}\, dS|_{\lambda=\mu=1}, \qquad (52)$$

$$\lim_{a\to\infty}\int \mathfrak{D}_\mu\mathfrak{L}_0\, dv|_{\lambda=\mu=1} = -\lim_{a\to\infty}\oint D^n\mathfrak{L}\, dS_{|\lambda=\mu=1}. \qquad (53)$$

We prove that identity (52) is a generalization of the virial theorem given by Robinson and Hirschfelder[9] and that identity (53) leads, by specialization, to the various identities derivable from Kato identity.[3,2] From (11), we have

$$\lim_{a\to\infty}\oint D^n\mathfrak{L}\, dS|_{\lambda=\mu=1} = \lim_{a\to\infty}\oint\left[\frac{\delta\mathfrak{L}}{\delta U_{,r}}\frac{\partial U}{\partial\tau} + \frac{\delta\mathfrak{L}}{\delta U_{,rr}}\frac{\partial}{\partial r}\left(\frac{\partial U}{\partial\tau}\right)\right]_{\lambda=\mu=\tau=1} dS + \lim_{a\to\infty}\oint\left[\frac{\delta\mathfrak{L}}{\delta V_{,r}}\frac{\partial V}{\partial\tau} + \frac{\delta\mathfrak{L}}{\delta V_{,rr}}\frac{\partial}{\partial r}\left(\frac{\partial V}{\partial\tau}\right)\right]_{\lambda=\mu=\tau=1} dS, \qquad (54)$$

where V is the Green's function of the adjoint problem defined as a planewave incident in direction $-\mathbf{k}_f$ and scattering into $-\mathbf{k}_i$. The derivatives should be evaluated in the following ways:

(a) $$\partial/\partial\lambda\, F(\lambda r, k/\lambda)|_{\lambda=1} = (r\,\partial/\partial r - k\,\partial/\partial k)F(r, k), \qquad (55)$$

where F is any function of r and k;

(b) $$\partial/\partial\lambda\, \Delta(\lambda r)|_{\lambda=1} = -2\Delta(r), \qquad (56)$$

with $\Delta(r)$ the Laplacian in spherical coordinates.

(1) We give now an example of Eq. (52). We have

$$\mathfrak{L}_0 = \tfrac{1}{2}V[-\Delta + \mathbf{V}(r) - k^2]U + \tfrac{1}{2}U[-\Delta + \mathbf{V}(r) - k^2]V \qquad (57)$$

and

$$\int \frac{\delta \mathfrak{L}_0}{\delta \lambda}\bigg|_{\lambda=1} dv = \frac{1}{2}\int V\left[2V(r) + r\frac{\partial V(r)}{\partial r}\right]V\, dv + \frac{1}{2}\int U\left[2V(r) + r\frac{\partial V(r)}{\partial r}\right]V\, dv. \quad (58)$$

On the other hand,

$$\lim_{\alpha\to\infty}\int D^n\mathfrak{L}_0|_{\lambda=1}\, dS = \lim_{\alpha\to\infty}\oint \frac{1}{2}\left[\frac{\delta\mathfrak{L}}{\delta U_{,r}}\frac{\partial U}{\partial \tau} + \frac{\delta\mathfrak{L}}{\delta U_{,rr}}\frac{\partial}{\partial r}\left(\frac{\partial U}{\partial \tau}\right)\right]dS + \lim_{\alpha\to\infty}\oint \frac{1}{2}\left[\frac{\delta\mathfrak{L}}{\delta V_{,r}}\frac{\partial V}{\partial \tau} + \frac{\delta\mathfrak{L}}{\delta V_{,rr}}\frac{\partial}{\partial r}\left(\frac{\partial V}{\partial \tau}\right)\right]dS. \quad (59)$$

Using the reciprocity principle, $V(\mathbf{r} \mid \mathbf{r}_1) = U(\mathbf{r}_1 \mid \mathbf{r})$ and self-adjointness, Eq. (59) reads

$$\lim_{\substack{\mathbf{r}_1\to k_f\alpha\\ \mathbf{r}_0\to -k_i\alpha\\ \alpha\to\infty}}\int U(\mathbf{r}_1 \mid \mathbf{r})\left[2V(r) + r\frac{\partial V(r)}{\partial r}\right]U(\mathbf{r} \mid \mathbf{r}_0)\, dv = \oint\left[\psi_f\frac{\partial^2\psi_i}{\partial r\,\partial\tau} - \frac{\partial\psi_f}{\partial r}\frac{\partial\psi_i}{\partial\tau}\right]dS, \quad (60)$$

a result identical to the generalization of the Robinson–Hirschfelder theorem (Eqs. 31 and 38 of Ref. 9). Introducing (47) into (60), we obtain

$$\lim_{\substack{\mathbf{r}_1\to k_f\alpha\\ \mathbf{r}_0\to -k_i\alpha\\ \alpha\to\infty}}\int U(\mathbf{r}_1 \mid \mathbf{r})\left[2V(r) + r\frac{\partial V(r)}{\partial r}\right]U(\mathbf{r} \mid \mathbf{r}_0)\, dv = 2\pi\frac{d}{dk}[kF(\pi-\gamma)], \quad (61)$$

where γ is the angle between k_i and k_f.

(2) We now give two examples of identity (53). Using a partial wave expansion

$$U(\mathbf{r}, \mathbf{r}_0) = \sum_0^\infty A_n P_l(\cos\theta)\phi_l(r)/r, \quad (62)$$

where the $\phi_l(r)$ are real solutions, zero at the origin, of

$$d^2\phi_l/dr^2 + [k^2 - 2mV(r) - l(l+1)/r^2]\phi_l = 0. \quad (63)$$

Therefore,

$$\mathfrak{L}_0 = \phi_l(r)\{d^2/dr^2 + [k^2 - 2mV(r) - l(l+1)/r^2]\}\phi_l(r). \quad (64)$$

The volume of integration is the line $0 \le r \le \infty$. Let us take first $p = l$,

then

$$\int \frac{\delta\mathfrak{L}_0}{\delta\mu}\bigg|_{\mu=1} dv = -(2l+1)\int_0^\infty \frac{\phi_l^2(r)}{r^2}\, dr \quad (65)$$

and

$$\lim_{\alpha\to\infty}\oint D^n\mathfrak{L}_0\, dS = \lim_{R\to\infty}\left(\phi_l\frac{\partial^2\phi_l}{\partial r\,\partial l} - \frac{\partial\phi_l}{\partial r}\frac{\partial\phi_l}{\partial l}\right)\bigg|_0^R \quad (66)$$

with R the radius of a large sphere.

We can use the asymptotic expansion

$$\phi_n(r) = \sin[kr - \tfrac{1}{2}l\pi + \eta(k, l)]/k \quad (67)$$

and $\oint D^n\mathfrak{L}_0\, dS = -(\partial\eta/\partial l - \pi/2)/k$, provided that $V(r)$ does not have a singularity worse than r^{-t} $(t < 2)$. Therefore

$$(2l+1)\int_0^\infty \phi_l^2(r)/r^2\, dr = \left[\frac{\pi}{2} - \partial\eta(k, l)/\partial l\right]/k \quad (68)$$

is another Robinson–Hirschfelder equality. As a second example, we assume $p = R$, where R is the radius of a cut-off potential $V(r, R)$.

Let $V(r, R) = V_0(r)[1 - H(r-R)]$, where $H(x) = 1$ for $x > 0$ and $H(x) = 0$ for $x \le 0$. Therefore,

$$\int \frac{\delta\mathfrak{L}_0}{\delta\mu}\bigg|_{\mu=1} dv = -2m\int_0^\infty \phi_l^2(r)V_0(r)\,\delta(r-R)\, dr = -2m\phi_l^2(R)V_0(R). \quad (69)$$

However, the exact wavefunction outside R is known as

$$\phi_l(r) = r[j_l(kr) - \tan(\eta)\cdot n_l(kr)] \quad (70)$$

and

$$\int \frac{\delta\mathfrak{L}_0}{\delta\mu}\bigg|_{\mu=1} dv = -2mV_0(R)R \times [j_l(kR) - \tan\eta\cdot n_l(kR)]^2. \quad (71)$$

Since

$$\oint D^n\mathfrak{L}_0\, dS = \left(\phi_l\frac{\partial^2\phi_l}{\partial r\,\partial R} - \frac{\partial\phi_l}{\partial r}\frac{\partial\phi_l}{\partial R}\right)\bigg|_0^R = \frac{1}{k}\frac{\partial\tan\eta_l}{\partial R}, \quad (72)$$

we have

$$\partial\tan\eta_l/\partial R = -2mV_0(R)R \times [j_l(kR) - \tan\eta\cdot n_l(kR)]^2, \quad (73)$$

an often-derived Ricatti-type nonlinear differential equation.[3,14,15]

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The Existence of Closed Magnetic Surfaces*

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A toroidal vacuum magnetic field, which has closed magnetic surfaces in the neighborhood of the magnetic axis, is mathematically constructed. The existence of these surfaces is demonstrated by the theorem of Moser on the stability of mappings which are perturbations of rotations whose rotation angle is a function of the radius (twist mapping).

INTRODUCTION

THE magnetic field studied in this paper is a mathematical expression constructed to satisfy Maxwell's equations. It is not constructed from a current distribution. However, it may be imagined that the fields exist inside current coils wound on a torus (Stellarator). The windings are such that there is a field line which closes on itself (magnetic axis). In the example of this paper, the components of the magnetic field perpendicular to the magnetic axis vanish quadratically in the neighborhood of the magnetic axis ($l = 3$).

The existence of the magnetic surfaces is proved by the stability of a mapping of a plane into itself with a fixed point. This mapping may be described in the following way: Let a plane intersect the magnetic axis in a point P. Let P' be a point in the plane in the neighborhood of P. The image of P' is found by following a field line through P' until it returns to the plane in a neighborhood of P. Since P is on the magnetic axis and since the magnetic axis closes on itself, then P is its own image. If the mapping has invariant closed curves, then the field has closed magnetic surfaces generated by the closed curves moving along field lines.

If r, θ are the polar coordinates of a point in the plane, and r', θ' the image coordinates where $r = 0$ is the fixed point, then for the example, the mapping will be shown to be of the form

$$r' = r + r_1(r, \theta), \tag{1}$$

$$\theta' = \theta + \beta r^2 + \theta_1(r, \theta), \tag{2}$$

where the leading terms in r_1 are of the order r^4, the leading terms in θ_1 are of order r^3, and $\beta \neq 0$ is a constant. The mapping of Eqs. (1) and (2) is thus a perturbed twist mapping. The mapping will not possess closed invariant curves unless certain conditions are imposed upon r_1 and θ_1. The work of Moser[1,2] will be used to show that there is a neighborhood of the fixed point in which these conditions are satisfied.

Only an existence theorem is demonstrated so that the results may be of only theoretical interest. Thus, it will be shown that there is a magnetic field with a magnetic axis such that there exists a neighborhood of the magnetic axis which contains a magnetic surface. It does not follow that every point inside the magnetic surface will lie on a magnetic surface. However, as a neighborhood shrinks to the magnetic axis, the measure of the points in the neighborhood lying on magnetic surfaces approaches the total measure of the neighborhood.

I. UNITS AND COORDINATES

The symbols X, Y, Z denote the coordinates of a right-handed Cartesian system. In the X, Y plane there is a circle with its center at $Y = 0$, $X = R > 0$. The radius of the circle is less than R. A torus is generated by rotating this circle about the Y axis. The center of the circle generates a circle of radius R in the X, Z plane. A magnetic field is created inside the torus in such a way that the circle of radius R is a field line. This field line is the one chosen for the magnetic axis.

The symbols x and y are Cartesian coordinates of a plane containing the Y axis. The point $x = y = 0$ is the point of intersection of the magnetic axis with this plane. The x axis is in the X, Z plane while the y axis is parallel to the Y axis. The coordinate φ is the angular coordinate of the magnetic axis. It is chosen so that $X = R$ at $\varphi = x = 0$. As φ increases, a point on the magnetic axis makes a right-handed screw about the Y axis. The variables, x, y, φ are the coordinates to be used in the calculation. Their range is $-R \leq x < \infty$, $-\infty < y < \infty$, $0 \leq \varphi < 2\pi$.

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The relationship between the X, Y, Z and x, y, φ systems is given by

$$X = (R + x)\cos\varphi, \tag{3}$$

$$Y = y, \tag{4}$$

$$Z = -(R + x)\sin\varphi. \tag{5}$$

Note that x, y, φ are essentially cylindrical coordinates with $R + x$ the radial and y the axial variable.

The magnetic field is represented by the vector $\mathbf{B}$. Since $\mathbf{B}$ is a static vacuum field, it may be represented as the gradient of a scalar Ψ so that

$$\mathbf{B} = \nabla\Psi. \tag{6}$$

For a simple toroidal field in the positive φ direction, $\Psi = B_0R\varphi$ where B_0 is the magnitude of $\mathbf{B}$ at the radius R. No generality is lost if it is assumed that $B_0 = 1$ and $R = 1$.

A field whose scalar potential is ψ is superimposed on the simple toroidal field. Since $x = y = 0$ on the magnetic axis, then for this value of x and y, $\nabla\psi = 0$. The potential Ψ of the total field may be written

$$\Psi = \varphi + \psi. \tag{7}$$

The equation satisfied by ψ is $\nabla^2\psi = 0$, which in these coordinates may be written

$$\partial^2\psi/\partial x^2 + (1 + x)^{-1}\,\partial\psi/\partial x + \partial^2\psi/\partial y^2 + (1 + x)^{-2}\,\partial^2\psi/\partial\varphi^2 = 0. \tag{8}$$

The equations for the field lines are given by

$$dx/d\varphi = [(1 + x)^2(\partial\psi/\partial x)](1 + \partial\psi/\partial\varphi)^{-1}, \tag{9}$$

$$dy/d\varphi = [(1 + x)^2(\partial\psi/\partial y)](1 + \partial\psi/\partial\varphi)^{-1}. \tag{10}$$

II. CONSTRUCTION OF THE MAPPING

If in Eq. (8) ψ is replaced by $N_{n\alpha}(x)e^{i(ay+n\varphi)}$ and the equation multiplied through by $(1 + x)^2e^{-i(ay+n\varphi)}$, the result is

$$(1 + x)^2d^2N_{n\alpha/dx^2} + (1 + x)\,dN_{n\alpha/dx} - [\alpha^2(1 + x)^2 + n^2]N_{n\alpha} = 0. \tag{11}$$

If I_n and K_n are modified Bessel functions of the first- and second-kind, respectively, then $I_n[\alpha(1 + x)]$ and $K_n[\alpha(1 + x)]$ are solutions of Eq. (11). The functions $N_{n\alpha0}(x)$ and $N_{n\alpha1}(x)$ will be defined by

$$N_{n\alpha0}(x) = \frac{K_n'(\alpha)I_n[\alpha(1 + x)] - I_n'(\alpha)K_n[\alpha(1 + x)]}{K_n'(\alpha)I_n(\alpha) - I_n'(\alpha)K_n(\alpha)}, \tag{12}$$

$$N_{n\alpha1}(x) = \frac{K_n(\alpha)I_n[\alpha(1 + x)] - I_n(\alpha)K_n[\alpha(1 + x)]}{\alpha[K_n(\alpha)I_n'(\alpha) - I_n(\alpha)K_n'(\alpha)]}. \tag{13}$$

The primes in Eqs. (12) and (13) denote differentiation with respect to the arguments of I_n or K_n and not with respect to x.

Since $N_{n\alpha0}$ and $N_{n\alpha1}$ are linear combinations of solutions to Eq. (11), they are themselves solutions to Eq. (11). From Eqs. (12) and (13), it is seen that

$$N_{n\alpha0}(0) = N_{n\alpha1}'(0) = 1, \tag{14}$$

$$N_{n\alpha0}'(0) = N_{n\alpha1}(0) = 0. \tag{15}$$

From Eqs. (11), (14), and (15), the Taylor expansions of $N_{n\alpha0}$ and $N_{n\alpha1}$ to the third order are

$$N_{n\alpha0}(x) = 1 + \tfrac{1}{2}[(n^2 + \alpha^2)x^2] - \tfrac{1}{6}[(3n^2 + \alpha^2)x^3] \cdots, \tag{16}$$

$$N_{n\alpha1}(x) = x - x^2/2 + (2 + n^2 + \alpha^2)x^3/6 \cdots. \tag{17}$$

From Eqs. (16) and (17), an $l = 3$ field will be constructed. Choosing α_1 and α_2 such that $\alpha_1 > \alpha_2 > 0$, then to the third order

$$\cos\alpha_1 yN_{n\alpha_1 1}(x) - \cos\alpha_2 yN_{n\alpha_2 1}(x) = \tfrac{1}{6}[(\alpha_1^2 - \alpha_2^2)x^3] - \tfrac{1}{2}[(\alpha_1^2 - \alpha_2^2)xy^2]. \tag{18}$$

Similarly, if α_3 and α_4 are chosen such that $\alpha_3 > \alpha_4 > 0$, then to third order

$$\alpha_3^{-1}\sin\alpha_3 yN_{n\alpha_3 0}(x) - \alpha_4^{-1}\sin\alpha_4 yN_{n\alpha_4 0}(x) = \tfrac{1}{2}[(\alpha_3^2 - \alpha_4^2)x^2y] - \tfrac{1}{6}[(\alpha_3^2 - \alpha_4^2)y^3]. \tag{19}$$

If the left-hand sides of Eqs. (18) and (19) are denoted by $U_n(\alpha_1, \alpha_2, x, y)$ and $V_n(\alpha_3, \alpha_4, x, y)$, respectively, then the potential ψ to be used in constructing the mapping is given by

$$\psi = \sin\varphi U_0(\alpha_1, \alpha_2, x, y) - \cos\varphi V_1(\alpha_3, \alpha_4, x, y). \tag{20}$$

From Eqs. (18), (19), and (20), it is seen that to the fourth order the function ψ has the form

$$\psi = Ax^3 - 3Dx^2y - 3Axy^2 + Dy^3 + Ex^4 + Fx^3y + Gx^2y^2 + Hxy^3 + Jy^4 + \cdots, \tag{21}$$

where

$$A = \tfrac{1}{6}[(\alpha_1 - \alpha_2^2)\sin\varphi], \tag{22}$$

$$D = \tfrac{1}{6}[(\alpha_3^2 - \alpha_4^2)\cos\varphi], \tag{23}$$

and the functions E, F, G, H, and J are linear combinations of $\sin\varphi$ and $\cos\varphi$.

From Eqs. (9), (10), and (21), the field-line equations to the third order are given by

$$dx/d\varphi = 3Ax^2 - 6Dxy - 3Ay^2 + (4E + 6A)x^3 + (3F - 12D)x^2y + (2G - 6A)xy^2 + Hy^3, \quad (24)$$

$$dy/d\varphi = 3Dx^2 - 6Axy + 3Dy^2 + (F - 6D)x^3 + (2G - 12A)x^2y + (3H + 6D)xy^2 + Ky^3 + \cdots . \quad (25)$$

The symbols x_0 and y_0 denote respectively $x(0)$ and $y(0)$. If $x(\varphi)$ and $y(\varphi)$ are expanded as power series in x_0 and y_0, then to the third order this may be written

$$x(\varphi) = x_0 + x_{20}x_0^2 + x_{11}x_0y_0^2 + x_{02}y_0^2 + x_{30}x_0^3 + y_{21}x_0^2y_0 + y_{12}x_0y_0^2 + y_{03}y_0^3, \quad (26)$$

$$y(\varphi) = y_0 + y_{20}x_0^2 + y_{11}x_0y_0 + y_{02}y_0^2 + y_{30}x_0^3 + y_{21}x_0^2y_0 + y_{12}x_0y_0^2 + y_{03}y_0^3, \quad (27)$$

where x_{20}, x_{11}, y_{20}, $\cdots$ are functions of φ. These functions vanish at $\varphi = 0$.

If Eqs. (26) and (27) are substituted into Eqs. (24) and (25), the equations for the variables x_{20}, x_{11}, $\cdots$ may be found by equating coefficients of powers of x_0 and y_0. It may be shown (see Appendix I) that to the third order all coefficients vanish at $\varphi = 2\pi$, except

$$-x_{21}(2\pi) = -x_{03}(2\pi) = y_{30}(2\pi) = y_{12}(2\pi) = 36\int_0^{2\pi} A(\varphi)\,d\varphi \int_0^{\varphi} d(\varphi')\,d\varphi'. \quad (28)$$

From Eqs. (22) and (23)

$$36\int_0^{2\pi} A(\varphi)\,d\varphi \int_0^{\varphi} D(\varphi')\,d\varphi' = \pi(\alpha_1^2 - \alpha_2^2)(\alpha_3^2 - \alpha_4^2). \quad (29)$$

If the right-hand side of Eq. (29) is denoted by β, then to the third order

$$x(2\pi) = x_0 - \beta y_0(x_0^2 + y_0^2) + \cdots , \quad (30)$$

$$y(2\pi) = y_0 + \beta x_0(x_0^2 + y_0^2) + \cdots . \quad (31)$$

If Eq. (31) is multiplied by $i(i^2 = 1)$ and added to Eq. (30), the result is

$$x(2\pi) + iy(2\pi) = (x_0 + iy_0)\exp i\beta(x^2 + y^2) + f(x_0, y_0), \quad (32)$$

where the leading terms in $f(x_0, y_0)$ are of fourth order x_0 and y_0.

By making the substitution $x_0 + iy_0 = r\exp i\theta$, $x(2\pi) + iy(2\pi) = r'\exp i\theta'$, Eq. (32) is put in the form of Eqs. (1) and (2) where the leading terms in $r_1(r, \theta)$ are of order r^4 and those of $\theta_1(r, \theta)$ are of the order r^3.

III. STABILITY OF THE MAPPING

Equations (1) and (2) in themselves do not prove that the mapping has closed invariant curves; thus, if $r_1(r, \theta) = \epsilon^2 r^4$, then the mapping is unstable no matter how small ϵ is. The stability of the mapping is demonstrated by the following theorem proved by Moser[3]:

Given a mapping

$$\rho' = \rho + \lambda^2\rho_2(\rho, \theta), \quad (33)$$

$$\theta' = \theta + \lambda^2[\xi(\rho) + \theta_2(\rho, \theta)], \quad (34)$$

where $1 \leq \rho \leq 2$, $0 < \lambda \leq 1$. The functions ρ_2 and θ_2 are periodic with period 2π in θ. If the mapping satisfies the conditions that

(1) Every closed curve enclosing the fixed point ($\rho = 0$) intersects its image, and

(2) There exists a constant $Q \geq 1$ such that

$$Q^{-1} \leq d\xi/d\rho \leq Q, \quad (35)$$

$$|d^{m_1}\xi/d\rho^{m_1}| + \left|\frac{\partial^{m_2+m_3}\rho_2}{\partial\rho^{m_2}\,\partial\theta^{m_3}}\right| + \left|\frac{\partial^{m_4+m_5}\theta_2}{\partial\rho^{m_4}\,\partial\theta^{m_5}}\right| < Q,$$

$$(m_1 \leq 333), (m_2 + m_3 \leq 333), (m_4 + m_5 \leq 333) \quad (36)$$

then there exists a δ, independent of the constant λ, such that if

$$|\rho_2| + |\theta_2| < \delta, \quad (37)$$

the mapping of Eqs. (33) and (34) has closed invariant curves in the annulus $1 \leq \rho \leq 2$.

To apply the theorem to the mapping of Eqs. (1) and (2), first let C be a closed curve about the fixed point and let C' be its image. Since C and C' both enclose the fixed point, the only way they cannot intersect is for C' to be inside the region bounded by C, or vice versa. Since the mappings of Eqs. (1) and (2) are generated by following field lines, it must be flux preserving. Thus, within the region bounded by C, there must be the same flux as that with the region bounded by C'. This is not possible if one of the curves is contained in the region bounded by the other. Consequently, the two curves must intersect. This demonstration has assumed that the component of the magnetic field perpendicular to the x, y plane does not change sign within C or C'. This will be true if C is in a sufficiently small neighborhood of the origin.

[3] The theorem presented here is a special case of theorem (3) in Ref. 1.

It may be shown[2] that there is a neighborhood of the fixed point where the mapping meets the other requirements of the small twist theorem by substituting $\lambda\rho = r$, $\lambda\rho' = r'$. This changes the mapping of Eqs. (1) and (2) into the form of Eqs. (33) and (34), where for $\lambda \leq r \leq 2\lambda$, $1 \leq \rho \leq 2$, $\xi(\rho) = \beta\rho^2$, and

$$\rho_2(\rho, \theta) = \lambda^{-3} r_1(\lambda\rho, \theta), \tag{38}$$

$$\theta_2(\rho, \theta) = \lambda^{-2} \theta_1(\rho, \theta). \tag{39}$$

Because the leading terms in $r_1(r, \theta)$ are of r^4 and those in $\theta_1(r, \theta)$ are of r^3, then

$$\lim_{\lambda \to 0} \rho_2(\rho, \theta) = \lim_{\lambda \to 0} \theta_2(\rho, \theta) = 0. \tag{40}$$

Because of Eq. (40) and no matter how small δ is, there is some value of λ for which Eq. (37) will be satisfied since δ is independent of λ. Equation (36) states that the derivatives of ρ_2 and θ_2 must be bounded up to order 333. That this is true follows from the fact that the Bessel functions are entire functions. Equation (35) will be satisfied provided that β does not equal zero. From Eq. (29), it is possible to choose the constants α_1, α_2, α_3, α_4, so that β does not vanish.

The conclusion is that the magnetic field whose potential is $\varphi + \psi$, where ψ is given by Eq. (20), has closed magnetic surfaces in some neighborhood of the magnetic axis.

As stated earlier in the paper, this result is only an existence theorem. Thus, no attempt will be made to estimate the constant δ. The result applies only to geometries similar to a Stellarator.

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APPENDIX

The equations for x_{20}, x_{11} $\cdots$ may be found by substituting Eqs. (26) and (27) into Eqs. (24) and (25) and equating coefficients of equal power of x_0 and y_0. The solutions of these equations involving only coefficients of the power of x_0 and y_0 up to these orders may be written

$$x_{20}(\varphi) = 3 \int_0^{\varphi} A(\varphi')\, d\varphi', \tag{A1}$$

$$x_{11}(\varphi) = -6 \int_0^{\varphi} D(\varphi')\, d\varphi', \tag{A2}$$

$$x_{02}(\varphi) = -3 \int_0^{\varphi} A(\varphi')\, d\varphi', \tag{A3}$$

$$y_{20}(\varphi) = -3 \int_0^{\varphi} D(\varphi')\, d\varphi', \tag{A4}$$

$$y_{11}(\varphi) = -6 \int_0^{\varphi} A(\varphi')\, d\varphi', \tag{A5}$$

$$y_{02}(\varphi) = 3 \int_0^{\varphi} D(\varphi')\, d\varphi', \tag{A6}$$

$$\begin{aligned} x_{30}(\varphi) = {} & 4 \int_0^{\varphi} E(\varphi')\, d\varphi' + 6 \int_0^{\varphi} A(\varphi')\, d\varphi' \\ & + 18 \int_0^{\varphi} A(\varphi')\, d\varphi' \int_0^{\varphi'} A(\varphi'')\, d\varphi'' \\ & + 18 \int_0^{\varphi} D(\varphi')\, d\varphi' \int_0^{\varphi'} D(\varphi'')\, d\varphi'', \end{aligned} \tag{A7}$$

$$\begin{aligned} x_{21}(\varphi) = {} & 3 \int_0^{\varphi} F(\varphi')\, d\varphi' - 12 \int_0^{\varphi} D(\varphi')\, d\varphi' \\ & - 18 \int_0^{\varphi} A(\varphi')\, d\varphi' \int_0^{\varphi'} D(\varphi'')\, d\varphi'' \\ & + 18 \int_0^{\varphi} D(\varphi')\, d\varphi' \int_0^{\varphi'} A(\varphi'')\, d\varphi'', \end{aligned} \tag{A8}$$

$$\begin{aligned} x_{12}(\varphi) = {} & 2 \int_0^{\varphi} G(\varphi')\, d\varphi' - 6 \int_0^{\varphi} A(\varphi')\, d\varphi' \\ & + 18 \int_0^{\varphi} A(\varphi')\, d\varphi' \int_0^{\varphi'} A(\varphi'')\, d\varphi'' \\ & + 18 \int_0^{\varphi} D(\varphi')\, d\varphi' \int_0^{\varphi'} D(\varphi'')\, d\varphi'', \end{aligned} \tag{A9}$$

$$\begin{aligned} x_{03}(\varphi) = {} & \int_0^{\varphi} H(\varphi')\, d\varphi' \\ & + 18 \int_0^{\varphi} D(\varphi')\, d\varphi' \int_0^{\varphi'} A(\varphi'')\, d\varphi'' \\ & - 18 \int_0^{\varphi} A(\varphi')\, d\varphi' \int_0^{\varphi'} D(\varphi'')\, d\varphi'', \end{aligned} \tag{A10}$$

$$\begin{aligned} y_{30}(\varphi) = {} & \int_0^{\varphi} F(\varphi')\, d\varphi' - 6 \int_0^{\varphi} D(\varphi')\, d\varphi' \\ & - 18 \int_0^{\varphi} D(\varphi')\, d\varphi' \int_0^{\varphi'} A(\varphi'')\, d\varphi'' \\ & + 18 \int_0^{\varphi} A(\varphi')\, d\varphi' \int_0^{\varphi'} D(\varphi'')\, d\varphi'', \end{aligned} \tag{A11}$$

$$y_{21}(\varphi) = 2\int_0^{\varphi} G(\varphi')\,d\varphi' - 12\int_0^{\varphi} A(\varphi')\,d\varphi' + 18\int_0^{\varphi} D(\varphi')\,d\varphi' \int_0^{\varphi'} D(\varphi'')\,d\varphi'' + 18\int_0^{\varphi} A(\varphi')\,d\varphi' \int_0^{\varphi'} A(\varphi'')\,d\varphi'', \quad \text{(A12)}$$

$$y_{12}(\varphi) = 3\int_0^{\varphi} G(\varphi')\,d\varphi' + 6\int_0^{\varphi} D(\varphi')\,d\varphi' - 18\int_0^{\varphi} D(\varphi')\,d\rho' \int_0^{\varphi'} A(\varphi'')\,d\varphi'' + 18\int_0^{\varphi} A(\varphi')\,d\varphi' \int_0^{\varphi'} D(\varphi'')\,d\varphi'', \quad \text{(A13)}$$

$$y_{03}(\varphi) = 4\int_0^{\varphi} J(\varphi')\,d\varphi' + 18\int_0^{\varphi} A(\varphi')\,d\varphi' \int_0^{\varphi'} A(\varphi'')\,d\varphi'' + 18\int_0^{\varphi} D(\varphi')\,d\varphi' \int_0^{\varphi'} D(\varphi'')\,d\varphi''. \quad \text{(A14)}$$

From Eq. (20), it follows that if $\gamma(\varphi)$ is any of the functions A, D, E, F, G, H, J, then

$$\int_0^{2\pi} \gamma(\varphi)\,d\varphi = 0. \quad \text{(A15)}$$

From Eqs. (22) and (23) it follows that

$$\int_0^{2\pi} A(\varphi)\,d\varphi \int_0^{\varphi} A(\varphi')\,d\varphi' = \int_0^{2\pi} D(\varphi)\,d\varphi \int_0^{\varphi} D(\varphi')\,d\varphi'. \quad \text{(A16)}$$

From Eq. (A15) and by integration by parts

$$\int_0^{2\pi} A(\varphi)\,d\varphi \int_0^{\varphi} D(\varphi')\,d\varphi' = -\int_0^{2\pi} D(\varphi)\,d\varphi \int_0^{\varphi} A(\varphi')\,d\varphi'. \quad \text{(A17)}$$

From Eqs. (A15) and (A16), the right-hand sides of Eqs. (A1) through (A16) all vanish at $\varphi = 2\pi$ with the exception of (A8), (A10), (A11), and (A13). These four equations, together with Eqs. (A15) and (A17), may be used to derive Eq. (28).

On the Dimer Solution of Planar Ising Models

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Derivations of the partition function of the Ising model on a general planar lattice L, which proceed via an associated dimer problem and use Pfaffians, are simplified by constructing a lattice L^{Δ} (the "terminal lattice" derived from an "expanded lattice" of L) for which (A) the allowed dimer configurations are in *one–one* correspondence with allowed Ising polygon configurations on L, and which (B) is *planar* if L is planar so that Kasteleyn's theorem may be used directly to construct the appropriate Pfaffian. This is in contrast to previous use of *non*planar associated dimer lattices for which the correspondence is *not* one–one, so that is has been necessary to prove a somewhat obscure "cancellation theorem."

1. INTRODUCTION

SINCE Onsager's famous solution of the Ising model on a plane rectangular lattice,[1] a number of alternative and simpler derivations have been discovered. One of the most straightforward of these derivations relates the Ising configurational problem[2] to the combinatorics of hard dimers[3,4] on a suitable associated lattice. This derivation, which has been expounded by Kasteleyn,[5,6] by Montroll,[7] and by Hurst and Green,[8] has the additional advantage of illuminating the problem as to why only *planar* Ising lattices are analytically solvable. The purpose of the present paper is to show how this approach can be simplified still further, and in a way that removes a residual obscurity concerning the significance of the *non*planarity of the associated dimer lattices which have been employed previously.[9]

The main steps in the dimer solution of the Ising problem are:

(*a*) The zero-field Ising model partition function $Z(T)$ for a lattice L, which has a bond for each interaction term $J_{ij}s_is_j$ between spins i and j, is expressed in terms of the generating function $\Upsilon(v_{ij})$ of configurations of "polygons" drawn on L according to the rules:

(i) the lattice bond (ij) in a polygon carries a weight

$$v_{ij} = \tanh K_{ij}, \qquad K_{ij} = J_{ij}/kT; \tag{1}$$

(ii) an *even* number of bonds r (including $r = 0$) meet at each site i of L.[2]

(*b*) The configurational problem for polygons on the lattice L is related to a dimer problem[3,4] on an associated lattice L^{Δ}. The corresponding dimer generating function $\Delta(w_{kl})$ counts all configurations in which:

(i) each bond (kl) of L and its two terminal vertices k, l can be occupied by a "dimer" of weight w_{kl} (related to the v_{ij}) and

(ii) each site k of L^{Δ} is occupied by one and only one dimer.

(*c*) By associating properly chosen signs with the weights, an antisymmetric matrix $\mathbf{A} = [a_{kl}]$, $a_{kl} = \pm w_{kl} = -a_{lk}$, is constructed whose Pfaffian[10] $\mathrm{Pf}(\mathbf{A})$ is equal to the required generating function.

(*d*) The determinant of $\mathbf{A}$ is evaluated asymptotically for large regular lattices in a straightforward way by using the cyclic (or almost cyclic) properties of $\mathbf{A}$.[2,7] In view of the basic result[10]

$$[\mathrm{Pf}\,(\mathbf{A})]^2 = \mathrm{Det}\,(\mathbf{A}), \tag{2}$$

this yields an asymptotic expression for the generating function $\Upsilon(v_{ij})$, and hence for the partition function $Z(T)$ and the limiting free energy per spin.

Now, in a fundamental theorem on the dimer problem, Kasteleyn[5,6] has shown that for an arbitrary planar lattice a single Pfaffian can be constructed which is exactly equal to the generating

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function of dimer configurations; in particular, each dimer configuration is counted with a positive sign. Conversely, for nonplanar lattices either many Pfaffians are required or, in general, some configurations are counted negatively.[5,6] However, following the original paper by Hurst and Green[11] (in which Pfaffians were first introduced for the Ising problem), the associated lattice L^{Δ} in step (*b*) has previously[5-8] been taken as the corresponding "terminal lattice" L^{T}, which, in general, is *non*-planar as illustrated for the square lattice in Fig. 1.[12,13] Furthermore, the correspondence between allowed polygon configurations on L and allowed dimer configurations on L^{T} is *not* one-one; rather, it is one-one for some configurations but one-many for others, as illustrated in Fig. 2 for a vertex of the square lattice. In view of the nonplanarity of L^{T}, Kasteleyn's dimer theorem *cannot* be used in step (*c*). If, nonetheless, one constructs the "best" possible single Pfaffian, one discovers that those dimer configurations, counted incorrectly with a negative sign, miraculously cancel the errors due to the lack of one-one correspondence with the polygon configurations, so that the latter are finally counted correctly, and the day is saved![14] Although it has been proved that this surprising cancellation

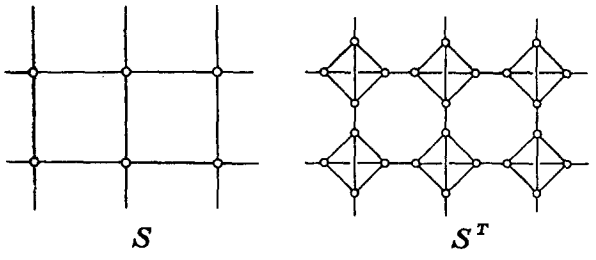

FIG. 1. Part of the square lattice S and its associated nonplanar terminal lattice S^{T}.

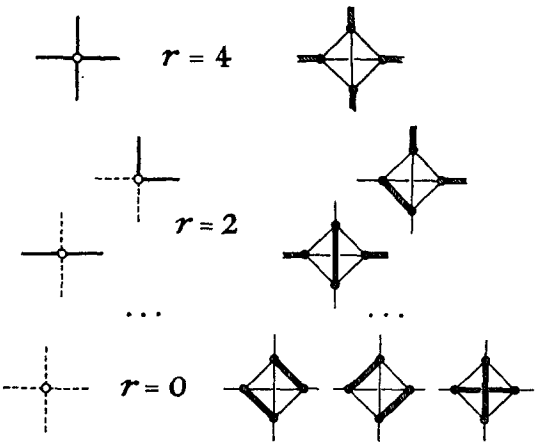

FIG. 2. Some allowed configurations of r polygon bonds at a vertex of the square lattice and their associated allowed dimer configurations on the terminal lattice illustrating the lack of one-one correspondence.

of miscounting with lack of correspondence can be arranged to hold for vertices of any degree, and hence applies to all planar Ising lattices,[8,15] the situation remains mysterious. Clearly, it would be more satisfactory if these rather inelegant complications could be avoided in all cases by the construction of an associated lattice L^{Δ} satisfying the conditions:

(A) polygon configurations on L are in *one-one* correspondence with dimer configurations on L^{Δ}, and

(B) L^{Δ} is a *planar* lattice (when L is planar) so that Kasteleyn's basic theorem may be employed directly to construct the appropriate Pfaffian.

As we show below, such a lattice can readily be found. It is the terminal lattice[12] of an "expanded lattice" L^{E}, constructed from L by "expanding" each vertex at which more than three bonds meet into a group of vertices of degree three (i.e., at which exactly three bonds meet).

2. EXPANDED LATTICES

The associated lattice $L^{\Delta} = (L^{E})^{T}$, which we eventually construct (see Fig. 6), could be introduced immediately, and one might then verify directly that it always satisfies the conditions (A) and (B). However, the general proof is a little simpler, and one obtains more insight into the problem if one proceeds in two stages. Firstly, we show that the partition function of the Ising problem on an arbitrary lattice L can always be derived from the partition function of an expanded lattice L^{E} in

[11] C. A. Hurst and H. S. Green, J. Chem. Phys. 33, 1054 (1960).

[12] The name "terminal lattice" has been introduced by Kasteleyn in Ref. 6. For a general lattice L the terminal lattice L^{T} is constructed by replacing a site i of L at which q_i bonds meet by a "city" or "cluster" of q_i sites one on the termination of each incident bond ("external" bond of L^{T}). These q_i sites are then joined by all possible "internal" bonds so that the city becomes a "complete graph" of order q_i.

[13] For the case of lattices with sites of *odd* coordination number, such as the honeycomb, the *augmented* terminal lattice L^{T+}, in which the city has an extra "dummy" terminal, has been proposed by Kasteleyn, or some equivalent device has been used (Ref. 8, pp. 207-9).

[14] What happens for the square lattice is that all configurations of dimers at a city are counted correctly except the last one shown in Fig. 2 where the dimers cross. This is counted with weight -1 so that the total weight of the $r = 0$ configuration is $1 + 1 - 1 = 1$ as required. For the triangular lattice, configurations of $r = 6$ and 4 bonds are in one-one correspondence, but for $r = 2$ and 0 the correspondence is one-three and one-fifteen, respectively! The details of the subsequent cancellation are thus more subtle.

[15] P. W. Kasteleyn (private communication).

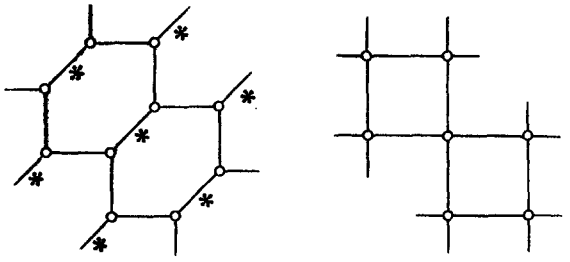

FIG. 3. Reduction of the honeycomb to the square lattice in the limit $K^* \to \infty$. The reverse transformation represents an "expansion" of the square lattice.

which no vertex has degree greater than three. Secondly, the precise equivalence with the dimer problem on the corresponding terminal lattice is demonstrated. Finally, it can be seen how the intermediate lattice L^E could be bypassed.

For convenience, we take the Ising partition function of an arbitrary lattice L to be

$$Z(T; L) = \sum_{s_i=\pm 1} \exp\left[\sum_{(ij)}^{(L)} K_{ij}(s_i s_j - 1)\right], \qquad (3)$$

where the first sum runs over the values $s_i = \pm 1$ for each vertex i in L and the second sum runs over all bonds in L. The interaction parameter K_{ij} is defined in (1) and is positive for ferromagnetic interactions which tend to align coupled spins. The inclusion of the term -1 in the exponent merely ensures that the zero of energy corresponds to the totally aligned state $s_i \equiv 1$ (all i). (If $K_{ij} \geq 0$ for all i, j, this will be the ground state, but otherwise it need not be.)

Now, observe that, if the limit $K_{ab} = K^* \to +\infty$ (or $J_{ab} = J^* \to \infty$) is taken for some pair of spins a and b linked by a "starred bond" in L, then these two spins become "locked" together, so that $s_a \equiv s_b$, since any terms in (3) with $s_a = -s_b$ include a factor $\exp(-2K^*)$ that approaches zero. Correspondingly, if a *set* of bonds in L is starred, we see that

$$\lim_{K^* \to \infty} Z(T; L) = Z(T; L^R), \qquad (4)$$

where L^R is the "reduced lattice" obtained from L by identifying all groups of sites $a, b, c, \cdots$ linked together by starred bonds and deleting the now redundant starred bonds. Perhaps the simplest instance of this reduction is the well-known relation between the honeycomb and the square lattices which is illustrated in Fig. 3.

Conversely, let us construct an "expanded lattice" L^E from L by replacing each vertex of degree $q \geq 4$ in L by a "cee" of $(q-2)$ vertices of degree three and $(q-3)$ extra "supplementary" bonds as shown in Fig. 4. (If one wishes to preserve some symmetry, one could alternatively use, here and below, a closed "ring" of q vertices and q supplementary bonds, although this entails the addition of more vertices and bonds than necessary.) It is evident that if L is a planar lattice then so is L^E. Furthermore, vertices of L^E have degrees one, two, or three only.

Now, consider the Ising problem on L^E in which each supplementary bond is assigned a parameter K^* while each "primary bond" has the parameter of the corresponding original bond in L. By Eq. (4) we then have

$$Z(T; L) = \lim_{K^* \to \infty} Z(T; L^E), \qquad (5)$$

so that quite generally one only needs to solve the Ising problem on lattices with vertices of degree three or less!

For completeness we now sketch step (a) of the general derivation. The identity

$$\exp(K_{ij} s_i s_j) \equiv \cosh K_{ij}\,[1 + v_{ij} s_i s_j], \qquad (6)$$

where $v_{ij} = \tanh K_{ij}$ holds for any variables $s_i s_j$ taking only the values ± 1. Introducing this expression into (3), expanding the products of factors $[1 + v_{ij} s_i s_j]$, and using

$$\sum_{s_i=\pm 1} (s_i)^r = \begin{cases} 2 & \text{for } r \text{ even}, \\ 0 & \text{for } r \text{ odd}, \end{cases} \qquad (7)$$

yields the well-known result

$$Z(T; L) = 2^N \Big[\prod_{(ij)} e^{-K_{ij}} \cosh K_{ij}\Big] \Upsilon(v_{ij}; L), \qquad (8a)$$

where N is the number of vertices of L (i.e., the number of spins) and

$$\Upsilon(v_{ij}; L) = \sum_{\Gamma(L)} \prod_{(gh) \subset \Gamma} v_{gh} \qquad (8b)$$

is the generating function of allowed polygon configurations $\Gamma(L)$, constructed on L according to the rules (ai) and (aii) stated in the Introduction, namely, if the bond (gh) occurs in the configuration $\Gamma(L)$ (which it does at most once) it carries

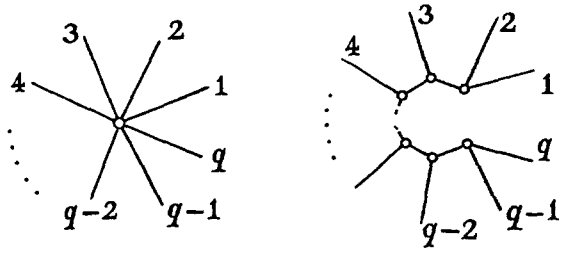

FIG. 4. The expansion of a general vertex of a lattice L into a "cee" of $q-2$ vertices of the "expanded lattice" L^E.

a weight factor v_{ab}, and in view of (7), an even number, r, of bonds meet at each vertex of L.

For polygon configurations on an expanded lattice L^E, we naturally assign a weight $v^* = \tanh K^*$ to each supplementary bond while each primary bond retains its original weight v_{ij}. The limit $K^* \to \infty$ in (5) may then be taken explicitly, and we obtain finally the general relation

$$Z(T; L) = 2^N[\prod_{(ij)}^{(L)} e^{-K_{ij}} \cosh K_{ij}] \times \Upsilon(v_{ij}, v^* = 1; L^E), \quad (9)$$

where the product runs only over the primary bonds of L^E (i.e., the original bonds of L). In obtaining the factor 2^N in (9), we have used the fact that, if N^* is the number of vertices of L^E and M^* the number of supplementary bonds, then $N^* - M^* = N$, since each supplementary bond can be associated with precisely one of the additional "cee" vertices, as may be checked in Fig. 4.

3. RELATION TO DIMER PROBLEM

To perform step (*b*) and relate the polygon configurations on L^E to a dimer problem, we now introduce the terminal lattice of L^E, namely, $L^\Delta = (L^E)^T$. This is constructed[12] by replacing each vertex of L^E of degree two by a pair of new vertices joined by an "internal bond" and replacing each vertex of degree three by a triplet of new vertices joined by a triangle of internal bonds (see Fig. 5). Evidently, this terminal lattice L^Δ will be planar if and only if L^Δ is planar. (This is, of course, the point of removing the vertices of higher degree from L.)

We now set up a *one–one* correspondence between polygon configurations on L^E and allowed dimer configurations on L^Δ [see, rules (*b*i) and (*b*ii) in the Introduction]. With the *presence* of any polygon bond on L^E, we associate the *absence* of a dimer on the corresponding "external bond" of L^Δ and vice versa.[16] By checking all the possible bond configurations at a vertex of degree 1, 2, or 3 in Fig. 5, one sees that the allowed dimer configuration on the internal bonds of L^Δ is always *unique* (in contrast to the Kasteleyn–Hurst–Green situation pictured in Fig. 2).

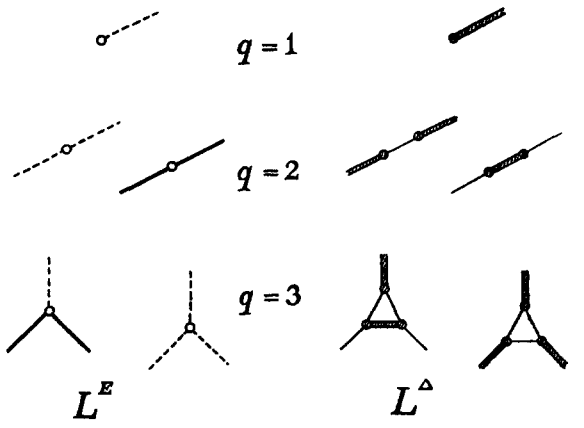

FIG. 5. Vertices of degree $q = 1$, 2, and 3 of L^E and their corresponding cities in the terminal lattice $L^\Delta = (L^E)^T$ showing the one–one correspondence of allowed bond and dimer configurations.

Suppose $\Delta(w_{ij}, w^*, w'; L^\Delta)$ is the generating function, defined in analogy to (8b), for dimer configurations on L^Δ in which (i) a dimer on an internal bond carries weight w', (ii) a dimer on an external bond carries weight w^* if it corresponds to one of the M^* supplementary (i.e., starred) bonds of L^E, but (iii) weight w_{ij} if it corresponds to a primary bond of L^E (i.e., to an original bond of L). To obtain the correct relative weights for the polygon configurations, we may put $w' = 1$ and must then set $w^* = 1/v^*$ and $w_{ij} = 1/v_{ij}$, since a polygon bond corresponds to the absence of a dimer. The dimer configuration in which all the external bonds of L^Δ are occupied then has weight $(v^*)^{-M^*}\Pi(v_{ij})^{-1}$. Since the corresponding polygon configuration on L^E has no bonds, it should have weight unity. Combining these observations we see that one–one correspondence is expressed by

$$\Upsilon(v_{ij}, v^*; L^E) = (v^*)^{M^*}[\prod_{(ij)}^{(L)} v_{ij}] \, \Delta(v_{ij}^{-1}, v^{*-1}, 1; L^\Delta). \quad (10)$$

Substitution in (9) yields the final identification of the Ising problem on L with the dimer problem on L^Δ, namely,

$$Z(T; L) = 2^N[\prod_{(ij)}^{(L)} v_{ij}(1 + v_{ij})^{-1}] \, \Delta(v_{ij}^{-1}, 1, 1; L^\Delta), \quad (11)$$

which completes step (*b*). (Note $v/(1+v) = e^{-K} \sinh K$.)

[16] In previous treatments, the presence of a polygon bond has been associated with the *presence* of a dimer, but our choice is simpler in general, since it avoids the need for extra "dummy" vertices at sites of L (or L^E) of odd degree (see Ref. 13).

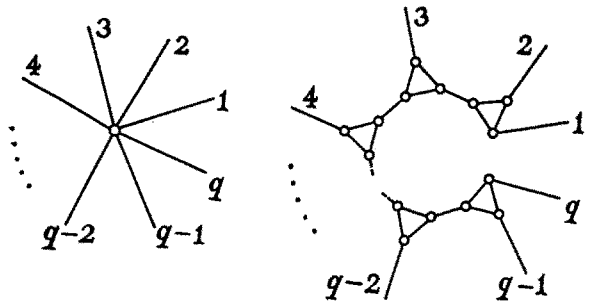

FIG. 6. Direct transformation of a general vertex of a lattice L to a "chain of triangles" on the associated dimer lattice L^{Δ} which is planar if L is planar.

If we perform the transformation to the terminal lattice on a general "cee" of L^{E} derived from a vertex of L of degree q (see Fig. 4), the net result is to replace the vertex by a "chain of $(q-2)$ triangles" as illustrated in Fig. 6. Altogether $3(q-2)$ vertices and $4q-9$ extra "secondary" bonds are introduced. Clearly, L^{Δ} is planar if (and only if) L is planar. One might now check directly that dimer configurations on the chain of triangles and their incident primary bonds are in one–one correspondence with polygon bond configurations at the vertex of the original Ising lattice L. Then the basic relation (11) could be written down directly from (8) without mention of L^{E}. The detailed verification of the direct transformation to L^{Δ} for a vertex of degree $q = 4$ is displayed in Fig. 7, which should be compared with Fig. 2. Our analysis via the expanded lattices assures us that this correspondence will be exact for any q if dimers on all the secondary bonds are assigned unit weight while those on the primary bonds are assigned the weights $w_{ij} = 1/v_{ij}$.

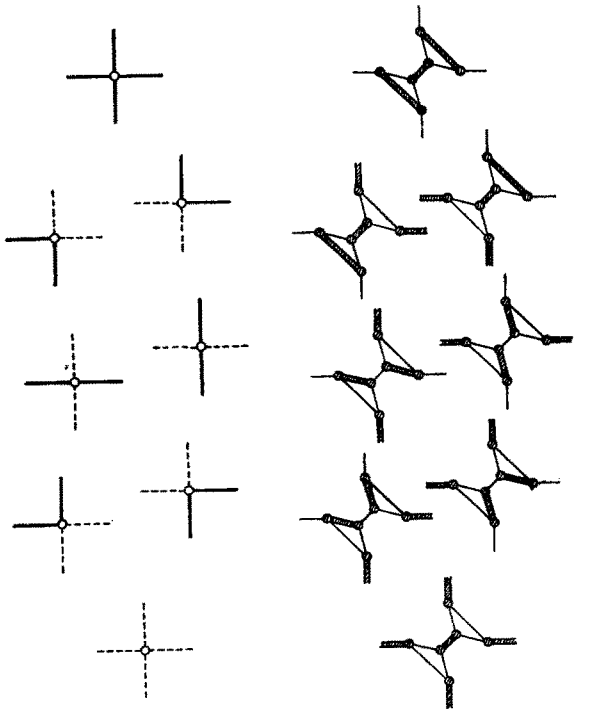

FIG. 7. Detailed verification of the one–one correspondence between polygon bond configurations at a vertex of degree 4 and dimer configurations on the corresponding chain of two triangles on L^{Δ}.

Evidently, for $q = 4$, the chain of triangles involves two more sites and one more bond than the corresponding terminal city. For $q \geq 6$, however, the number of bonds in the chain is the same as, or less than, in the corresponding city, although the number of points is, of course, always higher. This seems a small price to pay, however, for the simplicity of planarity and one–one correspondence.

4. REMAINING STEPS

For completeness we sketch the remaining steps (*c*) and (*d*) of the derivation although they are not new. To associate signs with the dimer weights w_{kl} and thereby construct an antisymmetric matrix $\mathbf{A} = [a_{kl}]$, we follow Kasteleyn[3,5,6] by *orienting* the bonds of the lattice L^{Δ} and adopting the convention: *if the arrow on a bond* (kl) *runs from vertex* k *to vertex* l, *the corresponding matrix element is* $a_{kl} = +w_{kl} = -a_{lk}$ *and vice versa.* [*Note* $a_{nn} \equiv 0$ *if there is no* (nn) *bond.*]

Now, for a planar oriented lattice embedded in the plane, we may define the "orientation parity" of a face to be "clockwise-odd" (or even) if the number of bonds in its perimeter (or "contour cycle") oriented in a clockwise sense is odd (or even). Kasteleyn's fundamental analysis[5,6] may then be summarized in the following theorem:

Theorem: Any planar lattice L^{Δ} can be oriented so that the orientation parity of each face is clockwise-odd and the Pfaffian $\mathrm{Pf}(\mathbf{A})$ of the corresponding antisymmetric matrix $\mathbf{A}$ is then equal to the generating function $\Delta(w_{kl})$ for dimer configurations on L^{Δ}.

The use of this theorem is demonstrated in Fig. 8 which displays a suitable orientation of the dimer lattice $S^{\Delta} = (S^{E})^{T}$ appropriate to the Ising problem on the rectangular lattice. Note that this is also the terminal lattice H^{T} of the honeycomb lattice! The clockwise-odd parity of each face is readily checked.

Using the labeling shown in Fig. 8 and the weights

$$w_1 = v_1^{-1}, \quad w_2 = v_2^{-1}, \quad \text{and} \quad w_3 = v^{*-1} = v_3^{-1} \tag{12}$$

required for the Ising model by (11) (but retaining $v_3 \neq 1$ so that the honeycomb Ising lattice can also be described), the matrix corresponding to Fig. 8 may be written in compact notation as

$$[\mathbf{A}]_{ij} = \begin{bmatrix} 0 & 1 & 1 & . & -w_1\omega_1^{-1} & . \\ -1 & 0 & 1 & . & . & -w_2\omega_2^{-1} \\ -1 & -1 & 0 & w_3 & . & . \\ . & . & -w_3 & 0 & 1 & 1 \\ w_1\omega_1 & . & . & -1 & 0 & 1 \\ . & w_2\omega_2 & . & -1 & -1 & 0 \end{bmatrix}, \tag{13}$$

where the factors $\omega_1^{\pm 1}$ and $\omega_2^{\pm 1}$ denote matrix elements in the blocks $(i \pm 1, j)$ and $(i, j \pm 1)$, respectively.

The construction of the matrix **A** completes step (*c*). To illustrate the final step in the derivation of the Ising partition function, we consider an $n \times m$ rectangular Ising lattice of $N = nm$ sites with interactions J_1 horizontally and J_2 vertically, and, at the same time, the corresponding honeycomb lattice of $2nm$ sites and interactions J_1, J_2, and J_3. By (11), (2), and Kasteleyn's theorem, the free energy per spin in the thermodynamic limit of an infinite lattice is

$$\begin{aligned} -F/kT &= \lim_{n,m\to\infty} (1/nm) \ln Z(T; L_{nm}) \\ &= 2 \ln 2 + \ln v_1v_2v_3 \\ &\quad - \ln (1 + v_1)(1 + v_2)(1 + v_3) \\ &\quad + \lim_{n,m\to\infty} \tfrac{1}{2} (1/nm) \ln \operatorname{Det} (\mathbf{A}_{nm}), \end{aligned} \tag{14}$$

where for the rectangular lattice we must put $v_3 = v^* = 1$.

Now the matrix **A** for this problem is cyclic in 6×6 blocks except for perturbations due to missing interactions at the edges of the lattice. (If periodic boundary conditions had been imposed, the lattice would no longer be planar and four Pfaffians would be needed to express the dimer generating function exactly.[3]) Since we are interested only in the value of $\operatorname{Det}(\mathbf{A}_{nm})$ for a large lattice, however, we may (rigorously) neglect the departures from strict periodicity and block diagonalize $\mathbf{A}_{nm}$ to sufficient approximation by the standard unitary transformation. The (r, s) block will have the form (13) with

$$\omega_1 = \exp [i\theta_1(r)], \qquad \omega_2 = \exp [i\theta_2(s)], \tag{15}$$

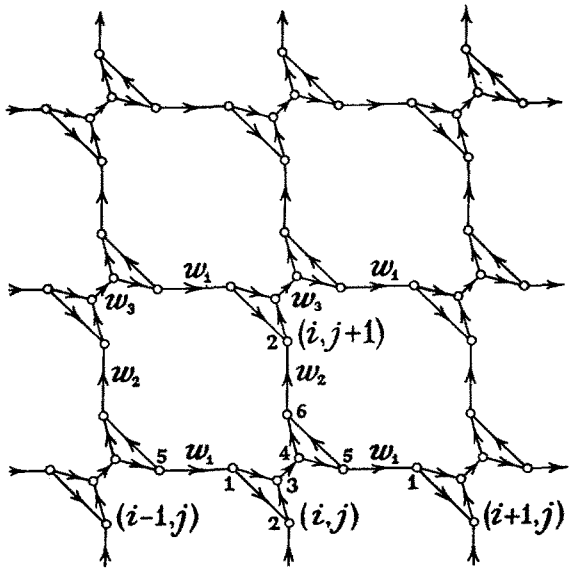

FIG. 8. The dimer lattice $L^{\Delta} = (S^{E})^{T} = H^{T}$ associated with the Ising problem on the square, S, and honeycomb lattice H, showing a suitable clockwise-odd orientation of the bonds.

where

$$\begin{aligned} \theta_1(r) &= 2\pi r/m, \qquad r = 1, 2, \cdots m, \\ \theta_2(s) &= 2\pi s/n, \qquad s = 1, 2, \cdots n. \end{aligned} \tag{16}$$

The logarithm of $\operatorname{Det}(\mathbf{A}_{nm})$ is then expressed as a sum of nm terms of the form $\ln \operatorname{Det}[\mathbf{A}_{nm}]_{rs}$. In the limit $n, m \to \infty$, the sum becomes an integral and we obtain the symmetrical result

$$\begin{aligned} -F/kT &= 2 \ln 2 - \ln (1 + v_1)(1 + v_2)(1 + v_3) \\ &\quad + \tfrac{1}{2}(2\pi)^{-2} \int_{-\pi}^{\pi} d\phi_1 \int_{-\pi}^{\pi} d\phi_2 \ln D(\phi_1, \phi_2, \phi_3), \end{aligned} \tag{17}$$

where $\phi_1 + \phi_2 + \phi_3 = 2\pi$ and

$$\begin{aligned} D(\phi_1, \phi_2, \phi_3) &= 1 + v_1^2v_2^2 + v_2^2v_3^2 + v_3^2v_1^2 \\ &\quad - 2(1 - v_1^2)v_2v_3 \cos \phi_1 - 2(1 - v_2^2)v_3v_1 \cos \phi_2 \\ &\quad - 2(1 - v_3^2)v_1v_2 \cos \phi_3. \end{aligned} \tag{18}$$

This may be checked against the known answer for the honeycomb lattice.[2,17] On putting $v_3 = 1$ the last term in (18) drops out and (17) is easily reduced to Onsager's famous formula for the square lattice, namely,

$$\begin{aligned} -F/kT &= \ln 2 - (J_1 + J_2)/kT \\ &\quad + \tfrac{1}{2}(2\pi)^{-2} \int_{-\pi}^{\pi} d\theta_1 \int_{-\pi}^{\pi} d\theta_2 \ln (\cosh 2K_1 \cosh 2K_2 - \sinh 2K_1 \cos \theta_1 - \sinh 2K_2 \cos \theta_2). \end{aligned} \tag{19}$$

ACKNOWLEDGMENT

The partial support of the National Science Foundation is gratefully acknowledged.

[17] Notice that we have computed the free energy per *pair* of honeycomb lattice sites.

High-Energy Behavior of Feynman Integrals with Spin. I*

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(Received 15 February 1966)

A method of determining the leading behavior of planar graphs for two-body processes in a spin-½–spin-1 conserved vector current theory is outlined. The leading behavior can be found by inspection. Coefficients of lower-order terms can be found explicitly. In a later paper we hope to use our methods together with analysis of nonplanar graphs to justify the Reggeization hypothesis in nth order.

INTRODUCTION

IT has been suggested by Gell-Mann *et al.*[1] that, in a conserved vector current theory of a nucleon interacting with a heavy vector meson, the nucleon lies on a Regge trajectory. It had previously been thought that there was no class of Feynman graphs, which, together with the Born term, generated a Regge-pole behavior at high energy. Gell-Mann *et al.*[1] verified to fourth order that the leading terms at high energy gave the correct contribution to the high-energy Regge-pole behavior. The work was extended to sixth order by Cheng and Wu.[2] The motivation for this series of papers is to develop sufficiently powerful techniques with which to study the nth order of the Reggeization problem. In this first paper, we will content ourselves with studying the high-energy behavior of planar meson–meson scattering graphs. This is the simplest case to study, since the traces of the integrand can be expressed as explicit scalar products of the momenta. We have the somewhat surprising result that all such graphs have a high-energy behavior of $t^2 \ln^b t$, where b is a positive integer dependent upon the topology of the graph. This is in contrast to the spinless case, where the exponent of t was also dependent upon the topology of the graph. We also find that renormalization has a significant effect on the high-energy behavior. In fact, for any specific order, the overall leading behavior is contributed by that graph with the maximum number of divergent subgraphs. As is well-known, the leading term for any specific order is of little importance, since as we will find in a later paper, the leading term is cancelled by terms from nonplanar graphs. It is the advantage of our method of analysis that we can pick out the important lower-order contributions as well as the leading term.

Throughout this paper we will denote the mass of the nucleon (meson) by $m_1(m_2)$. We will use the matrix $g_{00} = 1$, $g_{11} = g_{22} = g_{33} = -1$.

1. THE TOPOLOGY OF FEYNMAN INTEGRALS

We consider a planar meson–meson scattering graph G with r lines and l independent loops. We label the external mesons with index i ($i = 1, 2, 3, 4$), $i = 1, 2$, ($i = 3, 4$) corresponding to the incoming (outgoing) mesons. Meson (i) has four momentum p_i. Further, we denote the boundary of the graph joining the vertices of mesons i, j, by b_{ij}. It is along the boundaries b_{12}, b_{23}, b_{34} that we carry momenta p_1, $p_5 \equiv p_1 + p_2$, p_4.

Throughout the analysis, it will be convenient to consider the graph G drawn on a plane A which, in consequence, is divided into $l + 4$ disjoint areas, $A_j (j = 1, \cdots, l)$ and $B_j (j = 1, 4, 5, 6)$, such that

$$A = \bigcup_{j=1}^{l} A_j + \bigcup_{j} B_j.$$

The first l areas A_j lie within the boundary of the graph, and it is around the boundary of such an A_j that we run internal momentum k_j in a clockwise direction. The other four areas $B_j (j = 1, 4, 5, 6)$ are external to the graph, area B_j having as part of its boundary that boundary line of the graph carrying external momenta p_j, where p_6 is defined to be zero momentum. An example of a graph properly labeled is given in Fig. 1.

We wish to consider two forms of the Feynman integral F_G corresponding to the graph G. The first form derived from the Feynman prescription[3] is, as is well-known, an integral over the internal momenta of essentially the product of r meson and nucleon

* This work was supported in part through funds provided by the Atomic Energy Commission under Contract AT(30-1)-2098. Most of this work was carried out at the Department of Applied Mathematics and Theoretical Physics, University of Cambridge, England.

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[2] H. Cheng and T. T. Wu, Phys. Rev. 140, B465 (1965).

[3] R. P. Feynman, Phys. Rev. 76, 769 (1949).

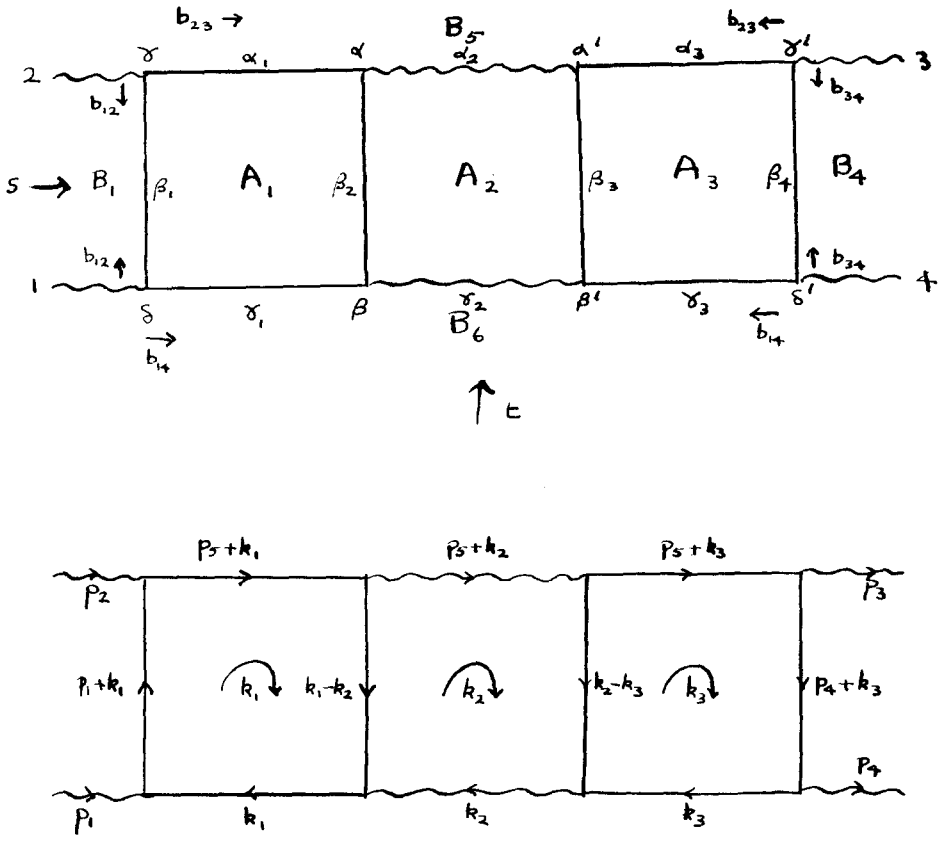


FIG. 1. The two-fermion loop graphs.

propagators. We will refer to this integral as I_G^1. Chisholm[4] transformed this expression for F_G into a form that explicitly exhibited F_G as a function of the invariants of the system. This was achieved by first introducing Feynman parameters and then integrating over the internal momenta. The final form for F_G is an integration over the Feynman parameters of a function of the Feynman parameters and the invariants and parameters of the system. We will denote this integrand by I_G^2. I_G^2 can be expressed in terms of two functions C and D[4,5] and certain derivations of these two functions. We will assume that the form and topological structure of these two functions are well-known. In particular, we can write D as an $(l+1) \times (l+1)$ determinant in the form

$$D = \begin{vmatrix} & & b_1 \\ & C & \vdots \\ & & b_l \\ \hline b_1, \cdots, b_l & & \theta \end{vmatrix}, \tag{1.1}$$

where $b_i (i = 1, \cdots, l)$ are linear functions of the external momenta of the problem p_1, p_4, p_5, the coefficients being linear functions of the Feynman parameters. b_i can be written down immediately from the momentum structure of the graph. We consider each of the r_i lines traversed by momentum k_i. Suppose the qth of these r_i lines carries a total momentum of $k_i - k_j + p_q$, where areas A_i and A_j have this line as a common boundary and p_q is the external momentum carried by this line, then $b_i = \sum_{q=1}^{r_i} \alpha_q p_q$, where α_q is the Feynman parameter for the qth line. For instance, for the graph of Fig. 1, $b_2 = \alpha_2 p_5$. θ is also a function of the parameters and momenta, but we will not be concerned with its structure.

We now wish to consider the derivations $X_i = (2C)^{-1}\partial D/\partial b_i$. As a determinant

$$X_i = \frac{1}{C} \begin{vmatrix} & & 0 \\ & C & 1 \\ & & 0 \\ \hline b_i, \cdots, b_l & & 0 \end{vmatrix}, \tag{1.2}$$

where all the entries in the final column are zero except the entry in the ith row which is unity. X_i

[4] J. S. R. Chisholm, Proc. Cambridge Phil. Soc. 48, 300 (1952).
[5] R. J. Eden, Phys. Rev. 119, 1763 (1960).

can thus be written as a sum over momenta p_1, p_4, p_5 and we define the coefficients by $X_i \equiv X_i^{p_1}p_1 + X_i^{p_4}p_4 + X_i^{p_5}p_5$. We will also need to study the double derivative $X_{ij} = (8C)^{-1}\partial^2 D/\partial b_i \partial b_j$. As a determinant

$$X_{ij} = \frac{1}{C}\left|\begin{array}{c|c|c} & & 0 \\ & C & 1 \\ & & 0 \\ \hline 0 \cdots 1 \cdots 0 & & 0 \end{array}\right|, \tag{1.3}$$

where the entries in the final row (column) are zero except for the entry in the jth column (ith row) which is unity. Before we specify the topological structure of these functions, we first define a partition from one area of the graph to another area of the graph as a continuous line in the plane A joining arbitrary points in the two areas. The partition only traverses lines of the graph and any line just once. Further, the partition enters any area at most once, and enters any B_i area only if one of the points to be connected lies in that area. We will refer to a partition from area B_1 to area B_4 as a t-partition.

We then have the prescription that $-X_{ij}C$ is equal to a sum of terms, there being a one-to-one correspondence between these terms and the partitions between area A_i and area A_j. Each term is the product of the Feynman parameters of the lines cut by the corresponding partition together with the C function for the graph, where the loops traversed by the partition have been omitted. We will refer to this derived graph as the fragment.

Similarly, $-X_i^{p_j}C$ is equal to a sum of terms, there being a one-to-one correspondence between these terms and the partitions between areas B_j and A_i. Each term is the product of the Feynman parameters of the lines cut by the corresponding partition together with the C function for the fragment.

These rules are easily derivable from explicit examination of the determinant. As an example, let us consider the graph of Fig. 1. We find $X_2^{P_1}C = -\beta_1\beta_2$ and $X_{13}C = -\beta_2\beta_3$.

The fact that I_G^2 can be expressed in terms of C, D, and X_i, X_{ij} functions can be seen from the following simple calculation. In the spinless case, the typical Feynman integral (F), takes the form

$$F = \int \prod_{i=1}^{r} d\alpha_i \int \prod_{j=1}^{l} d^4k_j [a_{ij}k_ik_j + 2b_ik_i + \theta]^{-r} \tag{1.4}$$

on the introduction of the r Feynman parameters α_i. The a_{ij} are the elements of the determinant C, each being a linear function of the Feynman parameters. Integrating over the internal momentum[4] we obtain

$$F = (i\pi^2)^l \frac{(r-2l-1)!}{(r-1)!} \int \prod_{i=1}^{r} d\alpha_i (C^{r-2l-2}/D^{r-2l}). \tag{1.5}$$

If, however, in the numerator we had, for instance, a factor $k_1 \cdot k_2$ then,

$$\begin{aligned} F' &\equiv \int \prod_{i=1}^{r} d\alpha_i \int \prod_{j=1}^{l} d^4k_j \frac{(k_1\cdot k_2)}{[a_{ij}k_ik_j + 2b_ik_i + \theta]^r} = [4(r-2)(r-1)]^{-1} \int \prod_{i=1}^{r} d\alpha_i \\ &\times \int \prod_{j=1}^{l} d^4k_j \left(\frac{\partial}{\partial b_1}\cdot\frac{\partial}{\partial b_2}\right)[a_{ij}k_ik_j + 2b_ik_i + \theta]^{-(r-2)} = \frac{(i\pi^2)^l}{4(r-2)(r-1)} \frac{(r-2l-3)!}{(r-3)!} \\ &\times \int \prod_{i=1}^{r} d\alpha_i \left(\frac{\partial}{\partial b_1}\cdot\frac{\partial}{\partial b_2}\right)(C^{r-2l-4}/D^{r-2l-2}) \\ &= (i\pi^2)^l \frac{(r-2l-1)!}{(r-1)!} \int \prod_{i=1}^{r} d\alpha_i \left[(X_1\cdot X_2)(C^{r-2l-2}/D^{r-2l}) + 4(-\tfrac{1}{2})(r-2l-1)^{-1}X_{12}(C^{r-2l-3}/D^{r-2l-1})\right]. \end{aligned} \tag{1.6}$$

Chisholm evaluated I_G^2 as a sum of terms. Specifically,

$$I_G^2 = \sum_{i=0}^{[\frac{1}{2}r_n]} A_i (C^{r-2l-2-i}/D^{r-2l-i}), \tag{1.7}$$

where $[\frac{1}{2}r_n]$ indicates the highest integer below $\frac{1}{2}r_n$ where r_n is the number of nucleon lines in the graph. The first term ($i = 0$) will be called the basic term. A_0 is derivable from I_G^1 in the following manner. Define the function $A \equiv I_G^1 \prod_1^r (Q_\mu^2 - m_i^2)$ where Q_μ is the total momentum carried by line μ; then A_0 is the same function of the $X_i (i = 1, \cdots, l)$ as A is of the variables k_i.

It is notationally convenient at this stage to introduce the functions Ω_μ, Ω'_μ, $\Omega_{\mu\nu}$. We define Ω_μ as

$$\Omega_\mu = \frac{1}{C}\left|\begin{array}{c|c|c} & & \epsilon_{\mu k_1} \\ & C & \vdots \\ & & \epsilon_{\mu k_l} \\ \hline b_1, \cdots, b_l & & P_\mu \end{array}\right|, \tag{1.8}$$

where the index μ refers to a particular line and

$\epsilon_{\mu k_i}$ is $+1$, -1, or zero depending on whether k_i appears in the expression for the momentum of the line μ with a positive or negative sign or does not appear at all. P_μ is the external momentum carried by the line μ. Thus, for a line carrying momentum $k_i - k_j + P_\mu$, $\Omega_\mu = X_i - X_j + P_\mu$. We further define Ω'_μ as $\Omega'_\mu = \gamma\cdot\Omega_\mu + m_1$. We can now restate the prescription for A_0 in terms of Ω'_μ. A_0 is the same function of the Ω'_μ's as A is of the variables $(\gamma\cdot Q_\mu + m_1)$.

$\Omega_{\mu\nu}$ is defined as the following determinant:

$$\Omega_{\mu\nu} = -\frac{1}{2C^2}\begin{vmatrix} & & \epsilon_{\mu k_1} \\ & C & \vdots \\ & & \epsilon_{\mu k_l} \\ \hline \epsilon_{\nu k_1} & \cdots \epsilon_{\nu k_l} & 0 \end{vmatrix}, \quad \text{if } \mu \neq \nu. \tag{1.9}$$

The second term ($i = 1$) in the Chisholm expansion of I_G^2 is itself a sum of terms, there being a one-to-one correspondence between these terms and distinct pairs of Ω''s. Each of these terms is derivable from the basic term by removing the corresponding pair of Ω''s and replacing with a pair of γ matrices γ^α, γ_α with a summation over α. Further, this term is multiplied by $\Omega_{\mu\nu} P$ when we remove Ω'_μ, Ω'_ν, where P is an operator acting on D in the following manner:

$$P(D^{-m}) = \int_0^\infty d\beta/[D + \beta]^m$$
$$= 1/(m-1)D^{m-1}, \qquad m \geq 2. \tag{1.10}$$

For the third term ($i = 2$) we remove two pairs of Ω''s, replace with γ matrices, sum and operate with $\Omega_{\mu_1\nu_1}\Omega_{\mu_2\nu_2}P^2$. The other terms in the expansion are obtained in an analogous manner.

As an example of this prescription, we will consider the graph of Fig. 2. Here,

$$I_G^1 = \frac{K[\bar{u}_3\gamma^\alpha[\gamma\cdot(P_5 + k_1) + m_1]\gamma^\beta u_2]\,[\bar{u}_4\gamma^\delta[\gamma\cdot(-k_1) + m_1]\gamma^\gamma u_1]\,g_{\alpha\delta}g_{\beta\gamma}}{[(P_5 + k_1)^2 - m_1^2][k_1^2 - m_1^2][(P_1 + k_1)^2 - m_2^2][(P_4 + k_1)^2 - m_2^2]}, \tag{1.11}$$

where K is a function of the parameters of the graph. The basic term of the Chisholm expansion is therefore

$$(i\pi^2)K(\bar{u}_3\gamma^\alpha\Omega'_{\alpha_1}\gamma^\beta u_2)(\bar{u}_4\gamma^\delta\Omega'_{\alpha_2}\gamma^\gamma u_1)D^{-2}, \tag{1.12}$$

where we index the lines with the Feynman parameter of the line. Thus $\Omega'_{\alpha_1} = \gamma\cdot(X_1 + P_5) + m_1$. The second and (in this case) the last term in the Chisholm expansion is

$$(i\pi^2)K(\bar{u}_3\gamma^\beta\gamma^\alpha\gamma^\delta u_2)(u_4\gamma_\beta\gamma_\alpha\gamma_\delta u_1)\Omega_{\alpha_1\alpha_2}g_{\alpha\delta}g_{\beta\gamma}D^{-1}. \tag{1.13}$$

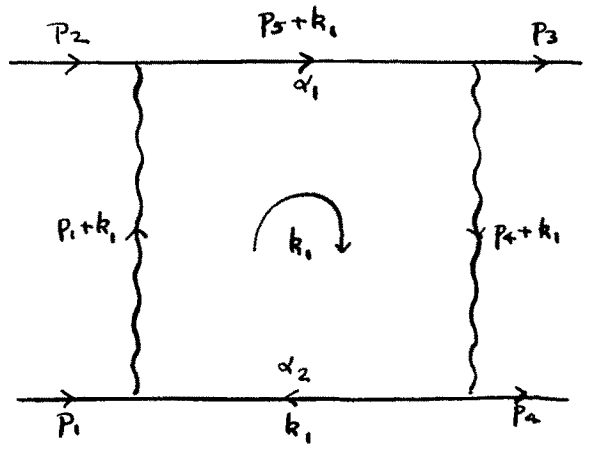


FIG. 2. A graph with a simple Chisholm expansion.

2. THE LEADING BEHAVIOR OF THE TWO-NUCLEON LOOP GRAPH

We wish to determine the leading behavior of the integral F_G (where G is the two-nucleon loop graph of Fig. 1) as the momentum transfer variable $t \equiv (p_1 - p_4)^2$ becomes large. For definiteness, we will consider that amplitude where all meson helicities are zero in the center-of-mass frame. Using the helicity vectors specified by Gell-Mann *et al*, [1] the polarization vectors e_1, $e_2(e_3, e_4)$ are linear sums over p_1 and $p_5(p_4$ and $p_5)$, where e_i is the polarization vector for meson (i). We argue in five steps.

A. Straddling

Let us consider first the basic term. If A_0 were unity, then we would have the spinless problem. The determination of the leading behavior[6-8] is then essentially equivalent to finding the maximum number of shortest paths through the graph connecting some vertex of the boundary line b_{23} with some vertex of boundary line b_{14}. The leading term of the Feynman integral in the limit of large t derives from successive integration over small neighborhoods of the origin of the sets of Feynman parameters of those lines in the shortest paths. To be specific, we intro-

[6] J. C. Polkinghorne, J. Math. Phys. **4**, 503, 1393 (1963).
[7] G. Tiktopoulos, Phys. Rev. **131**, 480 (1963).
[8] P. G. Federbush and M. T. Grisaru, Ann. Phys. (N. Y.) **22**, 263 (1963).

duce the scaling transformation of Federbush and Grisaru.[8] For a set of Feynman parameters $\alpha_i, \cdots, \alpha_{p+i}$, we transform to the variables $\rho, \bar{\alpha}_i, \cdots, \bar{\alpha}_{p+i}$ with the constraint $\sum_{i=i}^{p+i} \bar{\alpha}_i = 1$. ρ is termed the scaling parameter of the set and parametrizes the region of integration by planes parallel to the plane $\sum_i^{p+i} \alpha_i = 1$. Writing $D \equiv gt + h$ we define a d-line[9] as a set of Feynman parameters such that

(a) gh^{-1} is zero when these α's are set to zero.

(b) On transforming to the corresponding scaling variables, there remains a factor ρ^{d-1} in the numerator of the Feynman integral I_G^2 (in the spinless case, just the basic term with $A_0 = 1$) when we remove all overall factors from the C and D functions.

(c) d is minimal (d is termed the length of the set).

The integration is performed in the following $(p+1)$ stages:

(a) Of the set of d-lines take any d-line (d_1) not contained as a subset by any other d-line. Integrate over a small neighborhood of the origin of the α's of d_1, keeping only the lowest power of ρ_1, the scaling parameter of d_1, in g, h, and C.

(b) Let $\rho_1^{\beta+1}g_1$, $\rho_1^{\beta}h_1$, $\rho_1^{\beta}C_1$ be the g, h, C functions where only the lowest terms in ρ_1 have been kept. Let us relabel the original α's so that only the first $\theta_1\alpha$'s$(\alpha_1, \cdots, \alpha_{\theta_1})$ belong to d_1. Then g_1, h_1, C_1 are functions of $\bar{\alpha}_1, \cdots, \bar{\alpha}_{\theta_1}, \alpha_{\theta_1+1}, \cdots, \alpha_r$. Let us relabel these parameters as $\alpha_1, \cdots, \alpha_{\theta_1}, \alpha_{\theta_1+1}, \cdots, \alpha_r$. We now take any d-line (d_2) defined with respect to these new α's and new functions g_1, h_1, C_1 not contained as a subset by any other d-line defined with respect to these new α's and new functions g_1, h_1, C_1 and integrate over a small neighborhood of the origin of the α's of d_2 keeping only the lowest power of ρ_2, the scaling parameter of d_2, in g_1, h_1, C_1.

⋮

$(p+1)$. Let $\rho_p^{\gamma+1}g_p$, $\rho_p^{\gamma}h_p$, $\rho_p^{\gamma}C_p$ be the g_{p-1}, h_{p-1}, C_{p-1} functions in the approximation when only the lowest power of ρ_p has been kept. If there exist no more d-lines and p is maximal, then the leading behavior is extractable. In fact, we can apply the well-known integration formulas[7]

$$\text{(i)} \qquad \theta > d \int_0^1 \cdots \int_0^1 \frac{\rho_1^{d-1} \cdots \rho_M^{d-1}\, d\rho_1 \cdots d\rho_M}{(\rho_1 \cdots \rho_M gt + h)^{\theta}} \sim [(t)^{-d}(\ln t)^{M-1}][(g^d h^{\theta-d})^{-1}], \tag{2.1}$$

$$\text{(ii)} \qquad \theta = d^{(9)} \int_0^1 \cdots \int_0^1 \frac{\rho_1^{d-1} \cdots \rho_M^{d-1}\, d\rho_1 \cdots d\rho_M}{(\rho_1 \cdots \rho_M gt + h)^{\theta}} \sim \left[\frac{1}{t^d}(\ln t)^M\right]\left[\frac{1}{g^d}\right], \tag{2.2}$$

$$\text{(iii)} \qquad \theta < d \int_0^1 \cdots \int_0^1 \frac{\rho_1^{d-1} \cdots \rho_M^{d-1}\, d\rho_1 \cdots d\rho_M}{(\rho_1 \cdots \rho_M gt + h)^{\theta}} \sim \frac{1}{t^{\theta}} \int_0^1 \cdots \int_0^1 \frac{(\rho_1 \cdots \rho_M)^{d-\theta-1}}{g^{\theta}}\, d\rho_1 \cdots d\rho_M, \tag{2.3}$$

as t tends to infinity. The coefficients are necessarily convergent.

In the spin case, A_0 is a sum of scalar products $X_i \cdot X_j$. Each scalar product $X_i \cdot X_j$ is a linear sum over s, t, and m_i^2. Each scalar product $X_i \cdot X_j$ contributes an explicit t-factor. However, since the coefficient of t in $X_i \cdot X_j$ is a function of the Feynman paremeters, in general on scaling, powers of ρ are generated which raise the value of d and lower the leading behavior.

To discuss the problem in detail, we need to generalize the concept of d-line by relaxing the condition that d is minimal. We will refer to such a set as a t-set. Let us consider the effect on the numerator A_0 of scaling a t-set T. Let us consider that part of A_0 where the difference in the exponent (α) of t, and the exponent (β) of ρ is a maximum. If we have an overall factor $\rho^{\gamma-1}$ in the numerator when A_0 is replaced by unity, then we say the set T generates a leading behavior of $t^{(\alpha-\beta)-\gamma}$. Our problem is to find those t-sets that maximize $(\alpha-\beta)$-γ. As we will find in a later section, we need only consider those t-sets that divide the graph into three distinct, disjoint, connected regions—region R_0 within the boundary of the t-set, and regions R_1 and R_4 such that $\bigcup_{i=1} A_i = R_0 + R_1 + R_4$, and $R_1(R_4)$ has part of its boundary in common with the boundary $b_{12}(b_{34})$. Thus in the example of Fig. 1, if we scale loop 3, R_0 is A_3, R_1 is $A_1 + A_2$, and R_4 is empty. If A_i lies in $R_1(R_4)$ and A_j in R_0 or $R_4(R_0$ or $R_1)$, then the presence of the scalar product $X_i \cdot X_j$ in A_0 raises the leading behavior. This immediately follows from examination of the coefficient $X_i^{P_1}X_j^{P_4} + X_i^{P_4}X_j^{P_1}$ of $-\frac{1}{2}t$ in $X_i \cdot X_j$. On scaling, we find that $X_i^{P_1}X_j^{P_4}(X_i^{P_4}X_j^{P_1})$ is proportional to ρ^0 when A_i lies in $R_1(R_4)$. The second term is proportional to ρ or ρ^2. If both A_i

[9] I. G. Halliday, Ann. Phys. (N. Y.) 28, 320 (1964).

and A_j lie in R_1 or R_4, then, on scaling, the coefficient of t in $X_i \cdot X_j$ is found to be proportional to ρ. Therefore, if we say that a scalar product $X_i \cdot X_j$ straddles a t-set if all the partitions from area A_i to area A_j traverse at least one line of the t-set, (or if, when $i = j$, loop l_i lies in the scaling set), then it is only the scalar products that straddle the t-set that enhance the leading behavior for that t-set.

For the two-nucleon loop graph of Fig. 1, there are nine t-sets. For the four rungs β_1, β_2, β_3, β_4, the structure if the graph permits at most two straddling scalar products and hence, at most, a leading behavior of t. However, for the loops one and three, the structure of the graph permits at most four straddling scalar products and a possible leading behavior of t^2. Whether we can in fact find a term in A_0 with four straddling scalar products depends on the intricacies of the canceling mechanism in the trace calculation.

B. The Trace Calculation

We wish to calculate the trace of the matrix $X_{2b} \equiv (\gamma \cdot q_1)(\gamma \cdot q_2) \cdots (\gamma \cdot q_{2b})$. If $q_1 = q_2 = \cdots = q_{2b} = q$ then the relation $(\gamma \cdot q)(\gamma \cdot q) = q^2$ renders the calculation trivial. The trace is equal to $(q^2)^b$. If the trace involves only two momenta P_1, P_4, then the calculation is almost as simple. We have two possibilities. If the scalar products in X_{2b} are alternately $\gamma \cdot P_1$, $\gamma \cdot P_4$ then the trace is a power series in the scalar product $(P_1 \cdot P_4)$ of degree b. One can successively reduce the product X_{2b} by use of the anticommutation relations. In fact, we find that,

$$(\gamma \cdot P_4)(\gamma \cdot P_1)(\gamma \cdot P_4) = 2(P_1 \cdot P_4)(\gamma \cdot P_4) - P_4^2(\gamma \cdot P_1). \tag{2.4}$$

The trace calculation is thus reduced to the trace calculation of the matrix $(\gamma \cdot P_1)(\gamma \cdot P_4)$ or I, the traces in these two cases being $4P_1 \cdot P_4$ and 4, respectively. The coefficient of $(P_1 \cdot P_4)^b$ in the trace expansion is therefore 2^{b+1}. If the $(\gamma \cdot P_1)$, $(\gamma \cdot P_4)$ do not always occur alternately in X_{2b} then the highest power of $(P_1 \cdot P_4)$ in the trace expansion is less than b.

In our problem we are interested in only two momenta P_1, P_4, since it is only the product of P_1 with P_4 that gives rise to a t factor.

If in the matrix X_{2b}, momentum q_i^μ forms a scalar product with γ-matrix γ_μ, and γ_μ derives from a vertex (nucleon line) of the nucleon loop, then we say that q_i is associated with that vertex (nucleon line). For loop 3 of the example of Fig. 1, vertices γ' and δ' are necessarily associated with momentum P_4, since the important part of the meson polarization vectors is proportional to P_4. Further, vertices α' and β' must be associated with P_1 since it is the momentum X_i, where A_i lies in R_1, that provides the P_1 momentum. Hence, in the trace of loop 3 for the basic term, we cannot achieve alternating $(\gamma \cdot P_1)$, $(\gamma \cdot P_4)$ matrices, and therefore cannot achieve a t^2 behavior for loop 3 as a scaling set.

C. The Second Term in the Chisholm Expansion

If we examine that term in the coefficient A_1 of the Chisholm expansion, where we have replaced Ω'_{α_3}, Ω'_{γ_3} by γ matrices, then it is evident that we can effectively generate four straddling scalar products. This is because, on scaling loop 3, X_{33} generates a factor ρ^{-1} equivalent, so far as the high-energy behavior of the term is concerned, to a t factor in the numerator. The trace is certainly not zero, as can be seen by using the relation of Eq. (2.4) to simplify the product of the three γ-matrices associated with vertices α', β', and nucleon-line β_3, and again to simplify the product of the three γ-matrices associated with vertices γ', δ', and nucleon-line β_4. The relevant part of the trace is then,

$$4(P_1 \cdot P_4)^2 \operatorname{Tr}[(\gamma \cdot P_1)\gamma_\mu(\gamma \cdot P_4)\gamma^\mu]. \tag{2.5}$$

This derived trace is most simply calculated by moving the second γ^μ matrix to the left using the anticommutation relations and the relation $\gamma_\mu\gamma^\mu = 4I$. The coefficient of $(P_1 \cdot P_4)^3$, the highest power of $(P_1 \cdot P_4)$ in the trace expansion, is therefore -32. This is a particular case of the general result that the coefficient of $(P_1 \cdot P_4)^{b-1}$, the highest power of $(P_1 \cdot P_4)$ in the trace of the matrix $g^{\mu\nu}X_{2b}$, where

$$q_1 = q_3 = \cdots = q_{d-1} = q_{d+2} = \cdots = q_{2b-2} = P_1,$$

$$q_2 = q_4 = \cdots q_{d-2} = q_{d+1} = \cdots = q_{2b-1} = P_4$$

and

$$q_d^i = g_\mu^i, \qquad q_{2b}^j = g_\nu^j$$

is equal to $(-)2^{b+1}$.

The leading behavior of the third term of the Chisholm expansion of I_G^2 is therefore seen to be $t^2 \ln^2 t$ and derives from the integrand,

$$(-32)^2(P_1 \cdot P_4)^4 X_{11}X_{33}X_1^{P_1}X_4^{P_4}X_3^{P_1}X_3^{P_4}D^{-2}, \tag{2.6}$$

the scaling sets being loop 1 and loop 3.

D. Other Terms in the Chisholm Expansion

We immediately observe that there are other terms which have this leading behavior. For instance, if we replace the X_3 factors of β_3, β_4 by X_{33}, we lose

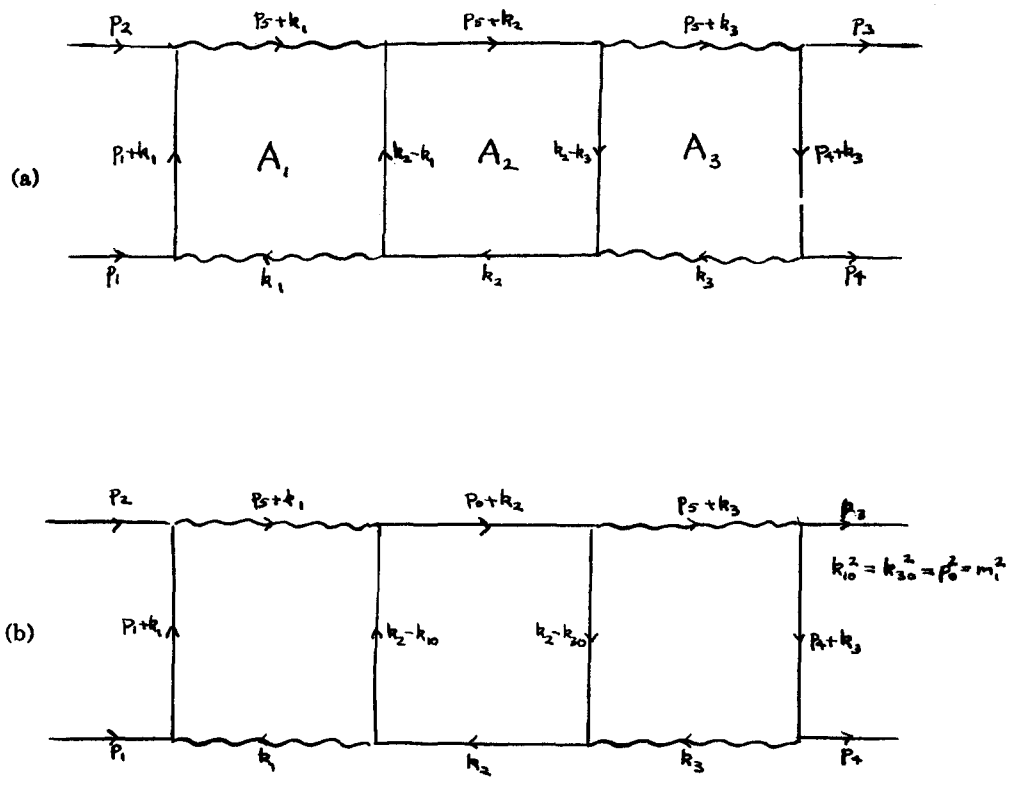


FIG. 3. Renormalization of a one-fermion loop graph.

an explicit t factor but gain a ρ^{-1} factor, an implicit t factor. The trace calculation again yields (-32). The term with two X_{33} factors and a leading behavior of $t^2 \ln {}^2t$ is therefore

$$-\tfrac{1}{2}(-32)^2 X_{33}^2 X_{11} X^{P_1} X_1^{P_4} (P_1 \cdot P_4)^3 C^{-1} D^{-1}. \quad (2.7)$$

Similarly,

$$-\tfrac{1}{2}(-32)^2 X_{11}^2 X_{33} X_3^{P_1} X_3^{P_4} (P_1 \cdot P_4)^3 C^{-1} D^{-1} \quad (2.8)$$

has a $t^2 \ln {}^2t$ behavior. It is easy to see that beside the term $X_{11}^2 X_{33}^2 (P_1 \cdot P_4)^2 C^{-2} P(D^{-1})$, which we consider in the section on renormalization, the only other term giving the $t^2 \ln {}^2t$ leading behavior is

$$-\tfrac{1}{2}(-32)^2 X_{11} X_{33} X_{13} X_1^{P_1} X_3^{P_4} (P_1 \cdot P_4)^3 C^{-1} D^{-1}. \quad (2.9)$$

E. Renormalization

We follow the Salam[10] procedure of subtracting from the original integral certain divergent integrals. The form of the integrand of the divergent subtraction integrals is identical to that of the original integral. The difference lies in the expression for the momentum of each line. Hence, these integrals can be expanded in the Chisholm manner as shown by Chisholm.[4]

[10] A. Salam, Phys. Rev. 82, 217 (1952).

We exhibit this procedure first for the graph of Fig. 3(a). To refer to this graph in the following analysis, we will use the symbol $G = 123$. The graph itself is not a divergent graph, but there exists a divergent subgraph, loop 2. Renormalization of the Feynman integral F_{123} is achieved by subtracting the Feynman integral $F_{123'}$, corresponding to the graph with the momentum labeling of Fig. 3(b). Since scalar products $k_1 \cdot k_2$, $k_3 \cdot k_2$ do not occur in the integrand $I^1_{123'}$ of $F_{123'}$, loop 2 is essentially isolated from the other two loops. Hence, we will find it convenient to write the Chisholm expansion of $I^2_{123'}$ as a product of the Chisholm expansion for loop 2, and loops 1 and 3. Specifically, we write $I^2_{123'} \equiv I^2_{13'} I^2_{2'}$. The Chisholm expansion of $I^2_{2'}$ consists of three terms, of which the last ($i = 2$) is undefined, since $P(D^{-1})$ is undefined. However, this last term can be written as $\ln [(D' + \alpha)D'^{-1}] \,|_{\alpha=\infty} = -[\ln \rho|_{\rho=0} + \ln D']$, where D' is the D function for the loop-2 graph. If we scale loop 2 and expand ρI^2_{123} in powers of ρ we find $\rho I^2_{123} = \sum_{n=0} \rho^n a_n$, where $a_0 = I^2_{13'}$. The only divergent part of I^2_{123} is the first term $a_0 \rho^{-1}$ and this is canceled by the term in the subtraction integral $F_{123'}$. Thus, to find the high-energy behavior of the term $T \equiv t^2 X_1^{P_1} X_3^{P_4} X_{22}^2 D^{-2}$ of I^2_{123}, we need to subtract off the first term of the

Taylor expansion in ρ, the scaling parameter for loop 2. The renormalized expression for T is then

$$T_R \equiv t^2 X_{22}^2 X_1^{P_1} X_3^{P_4} D^{-2} - t^2 X_{10}^{P_1} X_{30}^{P_4} \rho^{-4} D_0^{-2}, \quad (2.10)$$

where the suffix zero indicates the coefficient of the lowest power of ρ in the Taylor expansion for that function. The leading behavior derives from the part of T_R where only the lowest powers of ρ have been kept in X_1, X_3, X_{22}. We may then write this approximation (T_R') for T_R as

$$T_R' = \int_0^1 dx\, X_{10}^{P_1} X_{30}^{P_4} \frac{(-2) g t^3}{(gt\rho x + h)^3}, \quad (2.11)$$

where $D = \rho(gt\rho + h)$. The leading behavior for the term T_R is therefore $t^2 \ln t$ with scaling sets ρ and x. If we had blatantly ignored divergence problems and used the simple power counting methods used in previous sections we would find the leading behavior only $t^2(\ln t)^0$ with scaling set ρ. It is in this sense that we say renormalization raises the leading behavior. We must also consider the leading behavior of the remaining finite part of the subtraction integral $F_{123'}$, but this is easily seen to be t^2, since D_0 is independent of t.

Let us now consider the problem of renormalizing the Feynman integral F_0 of the graph of Fig. 1. First, we renormalize with respect to loop 3. For each divergent term in the Chisholm expansion we make a Taylor expansion, the first term being divergent. We represent F_0 pictorially as in Fig. 4, where the open circle represents the divergent term of F_0 and the shaded part the remaining finite part of F_0. As in the example of Fig. 3, we expand the renormalization subtraction term for loop 3(F_1) into a product of Chisholm expansions for loops 1, 2, and 3. That part of the subtraction term containing, as factor, the last term in the Chisholm expansion for loop 3, is divergent and cancels the loop-3 divergence in F_0. We can pictorially represent F_1 as in Fig. 4, where the shaded triangle represents the remaining finite part of F_1. To renormalize the loop-1 divergence in F_0 we subtract the loop-1 renormalization term

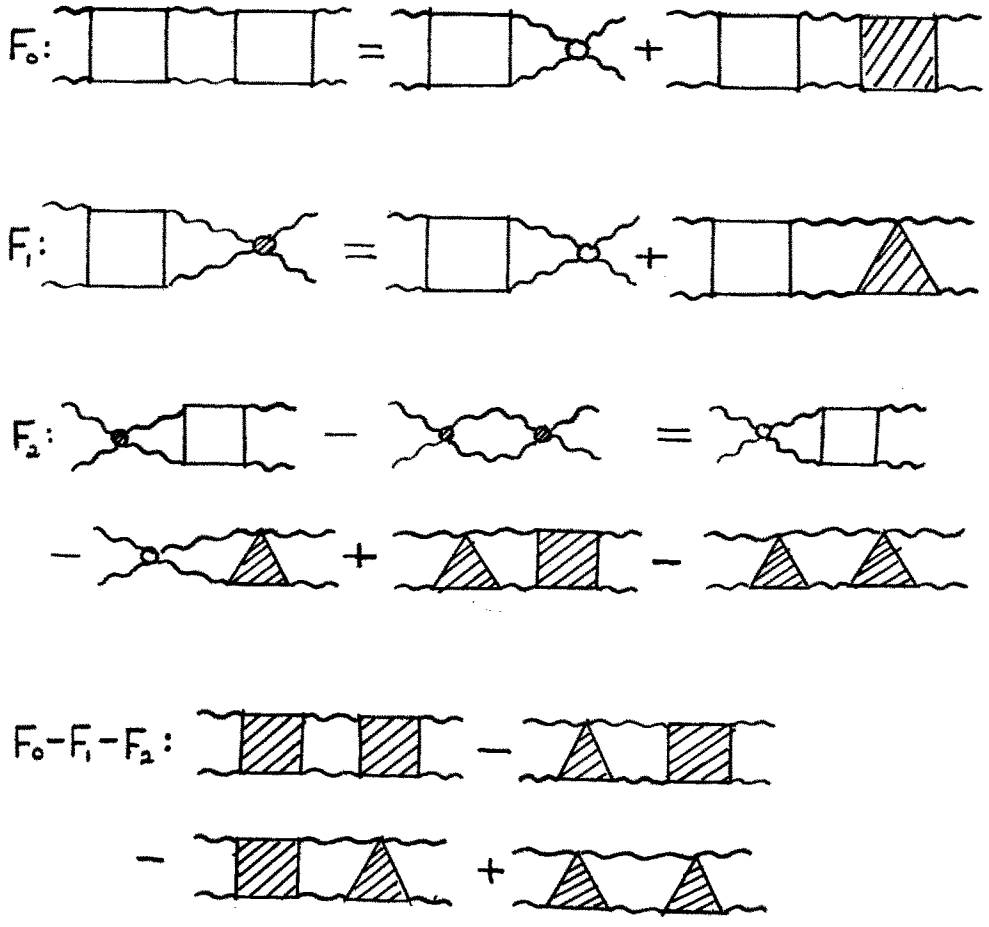


FIG. 4. Renormalization of the two-fermion loop graph.

(F_2) renormalized for loop 3 as represented in Fig. 4. Finally we must renormalize for the overall overlapping divergence; we subtract a renormalization term (F_3) renormalized for loops 1 and 3.

The only divergent term encountered was the last term in the Chisholm expansion of F_0. Suppose there were no divergent subgraphs, then the structure of the term would be $t^2C^{-2}\Pi X_{ij} \ln DD_0^{-1}$, where D_0 is the function D evaluated for particular values of s, t, say s_0, t_0. Expand $\ln DD_0^{-1}$ as

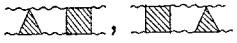
$$\ln (gt + h)h^{-1} - \ln (gt_0 + h_0)h^{-1}$$

and rewrite the first half of the integral as

$$t^2 \int_0^1 dx \int_0^1 \Pi\, d\alpha \frac{gt}{(gxt + h)} \left[\frac{1}{C^2} \Pi X_{ij}\right]. \qquad (2.12)$$

By the hypothesis, the function in the square brackets has a behavior at least ρ^0 in the scaling parameter for any subgraph. Here exists only one t-set of length one, namely x. The high-energy behavior of this term is therefore $t^2 \ln t$. If the only divergent subgraphs are logarithmically divergent subgraphs, which at the same time constitute t-sets, then the integral is still convergent, but the number of t-sets of length one is increased to $m + 1$, where m is the maximum number of such subgraphs consistent with the delta function constraints. The leading behavior of the last term in the Chisholm series for the two-number loop ladder (Fig. 1) is therefore $t^2 \ln {}^3t$.

We have found the leading behavior of only part of the renormalized integral $F_0 - F_1 - F_2 - F_3$, that part corresponding to the removal of the divergence in F_0. There are two other types of terms to evaluate at high energy.

(a) Terms 

The leading behavior is only t^2 since D is independent of t.

(b) Term  , which is again at most t^2. Finally, there is the finite part of the overall subtraction term to evaluate at high t. This is again at most t^2.

The leading behavior of the two-nucleon loop ladder is $t^2 \ln {}^3t$ deriving from the renormalized last term in the Chisholm expansion. It is not canceled by other terms in the expansion.

3. THE HIGH-ENERGY BEHAVIOR OF THE GENERAL PLANAR GRAPH

A. Nondivergent Terms in the Chisholm Expansion

We now generalize the results of the previous section to the case of general planar graphs of the meson–meson scattering process. For simplicity, we consider only those graphs such that:

(i) the nucleon loops have no inner structure—all meson lines joined to the loop are directed outward;
(ii) no meson line returns to the same nucleon loop.

We will later remove these restrictions. We calculate in the center-of-mass frame where the line defined by the 3-momentum vectors of the incoming particles is taken to be the three axis. The line defined by the outgoing 3-momentum vectors is taken to be in the 1-3 plane at an angle θ to the 3 axis. The energy will be denoted by w, the magnitude of the 3-momentum by q. The helicity vectors are defined as in Gell-Mann *et al.*[1]. For simplicity, we take all helicity values zero; the high-energy behavior is in fact independent of the helicity values.

Suppose the graph G has no divergent subgraphs, then, provided we can find a t-set such that:

(i) all the external lines of the t-set are meson lines;
(ii) no two external meson lines of the t-set are one and the same meson line;
(iii) the graph is divided by the t-set into only three distinct disjoint, connected regions—the region R_0 within the boundary of the t-set and region $R_1(R_4)$ having part of its boundary in common with boundary $b_{12}(b_{34})$;
(iv) there does not exist a meson line of the t-set that, when cut, separates the t-set into two distinct parts, but does not belong to a continuous path in the graph from boundary b_{23} to b_{14} lying entirely in the t-set;

the leading behavior is $t^2 \ln {}^bt$, where b is the maximum number of t-sets that can be scaled for any term of the Chisholm expansion, and that can fulfill the above four conditions. We will call such a t-set a T-set. If we cannot find a T-set, the behavior is $t^2 \ln t$. Before we attempt to justify this assertion, we introduce additional notation. If a vertex or nucleon line is associated with a $p_1(p_4)$ momentum vector, then we associate that point with an arrow pointing to the left (right). Further, we call the boundary between the region R_0 and $R_1(R_0$ and $R_4)$ the left (right) boundary of the T-set. Now, let us consider those nucleon loops of the T-set, T_1, adjacent to the left boundary of T_1. Order them from top to bottom. Consider the first loop (l_1). The external vertices on the left boundary must have arrows to the left. Let all other vertices have arrows

to the right. The arrow directions of the nucleon lines are determined by the fact that arrow directions must be alternating in the trace. Thus two nucleon lines must generate an X_{11} factor. Consider the next loop (l_2). The external vertices of the left boundary must have arrows to the left. Vertices connected to loop l_1 of necessity have arrows to the left. Let all other vertices have arrows to the right. The arrows of the nucleon lines are determined when two of them generate an X_{22} factor. The arrow directions of all other loops in the set are obtained by consistent use of this procedure, as they are also for the next row of loops. The procedure is consistent in that all vertex points in the right boundary have arrows to the right.

That the leading behavior of the term corresponding to the arrow system is t^2 on scaling the T-set follows from two assertions:

(i) the traces are nonzero,

(ii) the arrow system implies that to each internal and external meson line of the T-set we can associate a scalar product straddling the T-set.

Thus if,

e_M = number of external meson lines of the T-set,
e_N = number of external nucleon lines of the T-set,
i_M = number of internal meson lines of the T-set,
i_N = number of internal nucleon lines of the T-set,

and the number of lines (loops) in the set is $r_T(l_T)$, then $r_T = e_N + e_M + 3(l_T - 1)$. In our case $e_N = 0$. The number of straddling scalar products is $i_M + e_M = (l_T - 1) + e_M$. Thus the leading behavior of the T-set is t^a, where $a = -[e_M + 3(l_T - 1)] + [(l_T - 1) + e_M] + 2l_T$, namely two.

If b is the maximum number of T-sets, we can find, for any term of the Chisholm expansion, the leading behavior is $t^2 \ln {}^b t$, since the exponent α of the scaling parameters is always one less than the exponent β of D^{-1}. To prove this, suppose the T-set does not include external meson lines of the graph and that there are n fragments of the graph which, together with the T-set, makes up the graph. Let us label them $1, \cdots, i, \cdots, n$. If L is the total number of loops in the graph $3L + 1 = \sum r_i + r_T + e_M$, where $r_i = 3(l_i - 1) + e_{M_i}$ and $l_i(e_{M_i})$ are the number of loops (external meson lines) of the fragment i. Further $\sum e_{M_i} = 4 + e_M$. If $\gamma_i(\gamma_e)$ is the number of X_{ij} factors associated with the T-set (fragments of the graph), and E is the number of scalar products not straddling the T-set, then

$$\alpha = [3(l_T - 1) + e_M - 1] - [2l] + E - \gamma_i$$
$$= 1 - 4 + e_M + E - \gamma_i;$$

$$\beta = L + 1 - \gamma_i - \gamma_e$$
$$= \sum (l_i - 1) + 1 + e_p + 1 - \gamma_i - \gamma_e.$$

But $E + \gamma_e = \sum(i_{M_i} + e_{M_i}) - e_M = \sum(l_i - 1) + 4$, hence $\beta - \alpha = 1$. The same result holds if the T-set contains external particle vertices.

There are other terms, derived from this $t^2 \ln^b t$ term, that also have a leading behavior of $t^2 \ln^b t$:

(1) Suppose, in one of the loops (l_i) of the T-set, we remove two X_i factors to generate an X_{ii} factor, then the trace is nonzero if the two associated nucleon lines had opposite arrow directions. If they did not, then it is necessary to redirect the arrows of the intervening vertices and nucleon lines. This is not possible if this section of the loop corresponds to part of the boundary of the scaling set. However, if the procedure is possible, then in the new term α is decreased by one as is β. Hence $\beta - \alpha = 1$ still holds.

(2) If we remove two factors X_i, $X_j (i \neq j)$ then suppose,

(a) A_i lies in R_1, and A_j lies in R_4. If, in the original term,

(i) $X_i(X_j)$ contributed momentum $p_1(p_4)$, then in the rearrangement we lose a power of t and replace it with a power of ρ. Hence the leading behavior is reduced by two powers of t.

(ii) $X_i(X_j)$ contributed momentum $p_4(p_1)$, then in the rearrangement we lose a factor $\rho^2 t$ and gain a factor ρ, hence no change in behavior and no change in $\beta - \alpha$.

(b) Suppose A_i, A_j both lie in R_0, and suppose there exists a partition from A_i to A_j lying entirely within the T-set. Further, if $X_i(X_j)$ contributes a $p_1(p_4)$ or $p_4(p_1)$ momentum, then we lose a t factor but gain ρ^{-1} in the rearrangement. Hence neither the t^2 behavior nor $\beta - \alpha$ is changed.

(c) Similar arguments can be given for other arrangements of A_i, A_j in relation to the T-set.

We thus have the result that the leading behavior of any graph G, that has at least one T-set, is $t^2 \ln {}^b t$, where b is the maximum number of T-sets consistent with delta constraints and with compatible arrow configurations. There are many terms in the Chisholm expansion with this leading behavior but they are all derivable from a certain basic term that has a minimum number of X_{ij} factors; t-sets not satisfying the second, third, and fourth conditions for T-sets give a lower behavior than t^2.

We can easily remove the two restrictions placed on the set of planar graphs that we would consider. Suppose the T-set contains nucleon loops con-

tradicting the two restrictions. If we remove the offending meson lines and the nucleon loops, the problem of designating arrows has already been solved. Re-inserting the lines, any arrow conflict can be resolved by replacing the X_i functions of the two nucleon lines adjacent to the source of conflict by an X_{ij} function. The analysis is as before. The leading behavior from the finite terms of the Chisholm expansion is $t^2 \ln {}^b t$, where b is the number of T-sets consistent with delta-function constraints and with compatible arrow configurations.

B. Renormalization of the General Planar Graph

Suppose the graph G has p divergent subgraphs $S_1, \cdots, S_p$. We consider the question of renormalization and its effect upon the high-energy behavior of the graph under four headings. For the first three headings we consider all terms in the Chisholm expansion except the last term. Under the last heading we consider the last term in the Chisholm expansion.

1. *P Non-overlapping Logarithmically Divergent Subgraphs*

Consider a term T in the Chisholm expansion of I_G^2 that is divergent for q of these p divergent subgraphs. We denote this term by $T(\rho_1, \cdots, \rho_q)$ where ρ_i is the scaling parameter for the ith of the q subgraphs. Further, if we keep only the lowest power of the scaling parameters $\rho_{i_1}, \cdots, \rho_{i_r}$ in T and denote the derived term by

$$T(\rho_1, \cdots, \hat{\rho}_{i_1}, \cdots, \hat{\rho}_{i_2}, \cdots, \hat{\rho}_{i_r}, \cdots, \rho_q)$$

then we can write the renormalized term as

$$T_q(\rho_1, \cdots, \rho_q) \equiv \sum_{r=0}^{q} \sum_{i_r} (-1)^r \times T(\rho_1, \cdots, \hat{\rho}_{i_1}, \cdots, \hat{\rho}_{i_2}, \cdots, \hat{\rho}_{i_r}, \cdots, \rho_q), \tag{3.1}$$

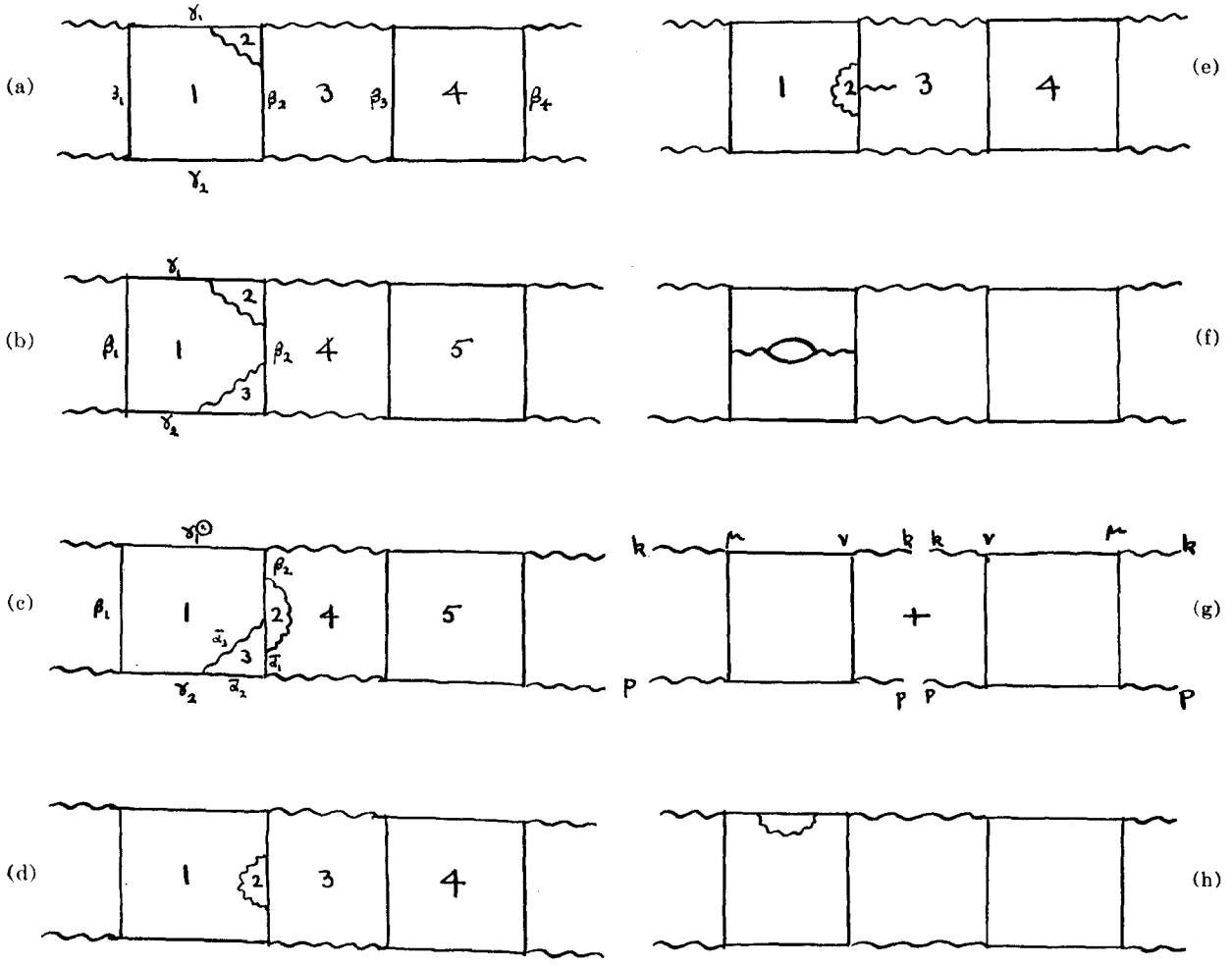


FIG. 5. Divergent graphs for the two-fermion loop graph.

where $\sum_{r}$, denotes a summation over all distinct sets of r scaling parameters. For the graph of Fig. 5(a), for example, we have the following divergent term in I_G^2:

$$t^4 \int_0^1 d\rho_2\, X_{11}X_{22}X_{44}X_1^{P_1}X_1^{P_4}X_4^{P_1}X_4^{P_4}\rho_2^2 D^{-2}, \qquad (3.2)$$

where ρ_2 is the scaling parameter for loop 2. For clarity we only specify the integration over ρ_2. To renormalize, we need to subtract a divergent term,

$$t^4 \int_0^1 d\rho_2\, \rho_2^{-1}X_{110}X_{440}X_{10}^{P_1}X_{10}^{P_4}X_{40}^{P_1}X_{40}^{P_4}D_0^{-2}, \qquad (3.3)$$

where the zero suffix on the functions in the integrand indicates the coefficient of the lowest power of ρ_2 in these functions. Writing $D \equiv \rho_2(A_1\rho_2 + A_0)$, where $D_0 = A_0$, we find the important part of the renormalized term can be written as

$$(-2)t^4 X_{110}X_{440}X_{10}^{P_1}X_{10}^{P_4}X_{40}^{P_1}X_{40}^{P_4} \times \int_0^1 d\rho_2 \int_0^1 dx_2 \frac{A_1}{(A_1\rho_2x_2 + A_0)^3}. \qquad (3.4)$$

The part we have ignored can easily be shown to have lower leading behavior. Renormalization therefore affects the term in two ways—it adds powers of $\rho_2 t$ to the numerator and replaces ρ_2 by $\rho_2 x_2$. Therefore, when we ignore the divergence of the term, the scaling sets giving the leading behavior are found by the simple counting methods outlined above. For every such scaling set involving ρ_2, we have an additional scaling set where we replace ρ_2 by x_2. Hence for the term (3.2) we have the scaling sets loop 4, $(\gamma_1\gamma_2\beta_1\beta_2\rho_2)$, $(\gamma_1\gamma_2\beta_1\beta_2x_2)$ and a leading behavior of $t^2 \ln {}^3t$.

As an example of a term with two divergences, let us consider the following term for the graph of Fig. 5(b).

$$T \equiv t^4 \int_0^1 d\rho_2 \int_0^1 d\rho_3 \times X_{11}X_{22}X_{33}X_{55}X_1^{P_1}X_1^{P_4}X_5^{P_1}X_5^{P_4}\rho_2^2\rho_3^2 D^{-2}, \qquad (3.5)$$

where $\rho_2(\rho_3)$ is the scaling parameter for loop 2 (loop 3). Renormalized for the divergent subgraph, loop 2, the term becomes

$$T_1 = (-2)t^4 \int_0^1 \int_0^1 d\rho_2\, d\rho_3\, \rho_3^{-1}X_{110}X_{550}X_{10}^{P_1}X_{10}^{P_4}X_{50}^{P_1}X_{50}^{P_4} \times \int_0^1 dx_2 \frac{(A_{11}\rho_3 + A_{10})}{[A_{11}(\rho_2x_2)\rho_3 + A_{10}(\rho_2x_2) + A_{01}\rho_3 + A_{00}]^3}, \qquad (3.6)$$

where $D \equiv \rho_2\rho_3(A_{11}\rho_2\rho_3 + A_{10}\rho_2 + A_{01}\rho_3 + A_{00}) \equiv D(\rho_2, \rho_3)$. We have again dropped some unimportant terms. Renormalized for both divergent subgraphs, loop 2 and loop 3, the term becomes

$$T_2 = (-2)(-3)t^4 \int_0^1 d\rho_2 \int_0^1 d\rho_3\, X_{110}X_{550}X_{10}^{P_1}X_{10}^{P_4}X_{50}^{P_1}X_{50}^{P_4} \int_0^1 dx_2 \int_0^1 dx_3\, A_{10}(A_{11}\rho_2x_2 + A_{01})/D^4(\rho_2x_2, \rho_3x_3) + (-2)t^4 \int_0^1 d\rho_2 \int_0^1 d\rho_3\, X_{110}X_{550}X_{10}^{P_1}X_{10}^{P_4}X_{50}^{P_1}X_{50}^{P_4} \int_0^1 dx_2 \frac{A_{11}}{D^3(\rho_2x_2, \rho_3)}. \qquad (3.7)$$

To express T_2 in a form symmetric in x_2 and x_3, we merely integrate by parts in x_2 the first part of the double integral. We then find,

$$T_2 = (-2)t^4\Big\{\int_0^1 d\rho_2 \int_0^1 d\rho_3\, X_{110}X_{550}X_{10}^{P_1}X_{10}^{P_4}X_{50}^{P_1}X_{50}^{P_4} \times \Big[\int_0^1 dx_2 \frac{A_{11}}{D^3(\rho_2x_2, \rho_3)} + \int_0^1 dx_3 \frac{A_{11}}{D^3(\rho_2, \rho_3x_3)} + (-3)\int_0^1 dx_2 \int_0^1 dx_3 \frac{[A_{10}A_{01} - A_{11}^2(\rho_2x_2)(\rho_3x_3)]}{D^4(\rho_2x_2, \rho_3x_3)} + (-1)\int_0^1 dx_2 \int_0^1 dx_3 \frac{A_{11}}{D^3(\rho_2x_2, \rho_3x_3)}\Big]\Big\}. \qquad (3.8)$$

The leading behavior is $t^2 \ln {}^4t$ arising from, for example, the four scaling sets loop 5, $(\gamma_1\gamma_2\beta_1\beta_2\rho_3\rho_2)$, $(\gamma_1\gamma_2\beta_1\beta_2\rho_3x_2)$, $(\gamma_1\gamma_2\beta_1\beta_2x_3x_2)$. We cannot scale $(\gamma_1\gamma_2\beta_1\beta_2x_3\rho_2)$ since this conflicts with delta function constraints.

We can immediately generalize these arguments into the following rule. To determine the leading behavior of a specific term in I_G^2, we first ignore divergences and look for those scaling sets that give leading behavior as determined by the simple power counting methods outlined in the first section. If such a scaling set contains r divergent subgraphs with scaling parameters $\rho_1, \cdots, \rho_r$ for that term and f denotes the remaining Feynman parameters of the set, then the 2^r sets

$$(\rho_1, \cdots, x_{i_1}, \cdots, x_{i_q}, \cdots, \rho_r, f),$$

where $1 \leq q \leq r$, and where we replace q of the ρ_i variables by the q corresponding x_i variables are also scaling sets. Because of delta function constraints, we can only scale $n + m$ sets, where n is the number determined by power counting methods and m is the number of distinct divergent subgraphs contained in the n scaling sets.

However, we must make the proviso that this rule is only true if there do not exist two of the r divergent subgraphs containing t-paths.[7] By t-path we mean a continuous path in the graph from boundary b_{23} to boundary b_{14}. As can be seen from the first part of the first integral of Eq. (3.7) that, if both divergent subgraphs contain t-paths, then there is no part of A_{10} and A_{01} proportional to t. The leading behavior of this renormalized term is therefore lower than that determined by power counting methods by a power of t. For the terms we are concerned with in planar meson-meson scattering graphs, only the last term in the Chisholm expansion is divergent for subgraphs containing t-paths.

2. *The General Case of p Logarithmically Divergent Overlapping and Non-overlapping Subgraphs*

The analysis is identical to that of the previous section. One first introduces the scaling parameters $\rho_1, \cdots, \rho_r$ for the r divergencies $(1 \leq r \leq p)$. One then renormalizes by introducing the additional parameters $x_1, \cdots, x_r$. The only difference is that now there are delta function constraints on those scaling parameters ρ_i that are overlapped by other divergences. However, the same rules with the same proviso still apply. For instance, the term for the graph of Fig. 5(c),

$$T \equiv t^4 \int_0^1 d\rho_2 \int_0^1 d\rho_3 \times X_1^{P_1} X_1^{P_4} X_5^{P_1} X_5^{P_4} X_{11} X_{22} X_{33} X_{55} \rho_2^2 \rho_3^2 D^{-2} \times \delta(\rho_2 + \bar{\alpha}_1 + \bar{\alpha}_2 + \bar{\alpha}_3 - 1), \tag{3.9}$$

where $\rho_2(\rho_3)$ is the scaling parameter for loop 2 (loops 2 and 3), is divergent for both the integrations ρ_2 and ρ_3. On renormalizing, we obtain a term similar in form to (3.7) and (3.8). The scaling sets for leading behavior are loop 5, $(\beta_1\beta_2\gamma_1\gamma_2\rho_3)$, $(\beta_1\beta_2\gamma_1\gamma_2 x_3)$, $(\beta_1\beta_2\gamma_1\gamma_2 x_2\bar{\alpha}_1\bar{\alpha}_2\bar{\alpha}_3)$ and leading behavior is $t^2 \ln {}^4t$.

3. *Linearly and Quadratically Divergent Subgraphs*

Let us first consider the graph of Fig. 5(d). In this case even the first term of the Chisholm expansion is undefined. In order to retain the Chisholm expansion method, we introduce the technique of Ward[11] as used by Chisholm.[4] We express, the nucleon self-energy part $N(p)$ in terms of a vertex part $\Lambda_\mu(p, p)$ with a zero external meson line. In fact, we write

$$N(p) = (-) \int_0^1 d\lambda\, (p - p_0)^\mu \Lambda_\mu(p^\lambda, p^\lambda), \tag{3.10}$$

where $p^\lambda = \lambda p + (1 - \lambda)p_0$, and p_0 is some 4-momentum on the mass shell. The renormalized self-energy part, $N^R(p)$, is then simply obtained by renormalizing the vertex part. Explicitly,

$$N^R(p) = (-) \int_0^1 d\lambda\, (p - p_0)^\mu \times [\Lambda_\mu(p^\lambda, p^\lambda) - \Lambda_\mu(p_0, p_0)]. \tag{3.11}$$

Similarly, for the meson self-energy divergence of Fig. 5(f), the Chisholm series is undefined. If $L_{\mu\nu}(p, p)$ denotes the Feynman integral for the meson–meson graph of Fig. 5(g) where $k = 0$, we can express the meson self-energy part $M(k)$ as

$$M(k) = \int_0^1 d\lambda_1 \int_0^{\lambda_1} d\lambda_2\, (k - k_0)^\mu \times (k - k_0)^\nu L_{\mu\nu}(k^\lambda, k^\lambda), \tag{3.12}$$

where $k^\lambda = \lambda k + (1 - \lambda)k_0$, and k_0 is on the mass shell.

To renormalize $M(k)$ we merely renormalize $L_{\mu\nu}$. Explicitly,

$$M^R(k) = \int_0^1 d\lambda_1 \int_0^{\lambda_1} d\lambda_2\, (k - k_0)^\mu (k - k_0)^\nu \times [L_{\mu\nu}(k^\lambda, k^\lambda) - L_{\mu\nu}(k_0, k_0)] \tag{3.13}$$

or

$$M^R(k) = \int_0^1 \mu_1\, d\mu_1 \int_0^1 d\mu_2\, (k - k_0)^\mu (k - k_0)^\nu \times [L_{\mu\nu}(k^{\mu_1\mu_2}, k^{\mu_1\mu_2}) - L_{\mu\nu}(k_0, k_0)]. \tag{3.14}$$

Thus to circumvent the problem of renormalizing self-energy parts, we consider equivalent graphs with self-energy parts replaced by vertex and meson–meson scattering parts. The Chisholm series is then well defined, and the divergences are only logarithmic. The Feynman integral for the original graph differs from the Feynman integral for the derived graph only in two respects. First, extra parameters (λ, μ) are introduced, and second, the product of the numerators of the two external nucleon (meson) lines of the self-energy part is changed from $(\gamma\cdot p + m)(\gamma\cdot p + m)$ [1] to $(\gamma\cdot p + m)(p - p_0)_\mu (\gamma\cdot p + m)$ $[(k - k_0)_\mu (k - k_0)_\nu]$, where $p[k]$ is the

[11] J. C. Ward, Phys. Rev. 77, 293 (1950).

external momentum of the self-energy part. We will denote this integral by $I_G^{1'}$. We can write the integral as an integral of $I_G^{2'}$ over the Feynman parameters and λ, where $I_G^{2'}$ is obtained from $I_G^{1'}$ by the same Chisholm rules that we obtained I_G^2 from I_G^1 when we define $\Omega_{\mu\mu}$ as

$$\Omega_{\mu\mu} = -\frac{1}{2C^2}\begin{vmatrix} C & \epsilon_{\mu k_1} \\ & \vdots \\ & \epsilon_{\mu k_l} \\ \hline \epsilon_{\mu k_1}, \cdots, \epsilon_{\mu k_l} & 0 \end{vmatrix}. \tag{3.15}$$

The analysis of the leading behavior is as before. It is evident that the additional parameters λ, μ_1, μ_2 can never belong to scaling sets giving leading behavior. For instance, renormalizing the term

$$T \equiv t^4 \int_0^1 d\rho_2\ \rho_2^2 X_{11}^2 X_{22} X_{44} X_1^{p_1} X_1^{p_4} X_4^{p_1} X_4^{p_4} D^{-2} \tag{3.16}$$

of Fig. 5(e) for the divergent loop 2, we find the numerator, after the introduction of the integration over x_2, contains a factor A_1 (see Eq. 3.4), the t part of which is proportional to λ^2.

By the rule of Sec. (3B1), the leading behavior of those terms in I_G^2, for the graphs of Fig. 5(d) and 5(f) divergent only for the self-energy parts, is $t^2 \ln {}^3t$.

The rule of Sec. (3B1), however, only holds for those m divergent subgraphs that are cut by at least one t-partition, since the A factors that appear in the numerator on renormalization must all have a part proportional to t. It is possible for a self-energy part not to be cut by any t-partition. For instance, for those terms in the Chisholm expansion, for the graph of Fig. 5(h) divergent only for the nucleon self-energy part, have a leading behavior at most $t^2 \ln {}^2t$.

4. *The Last Term in the Chisholm Expansion*

As explained in Sec. (2E), we consider the leading behavior of the expression,

$$t^3 \int_0^1 dx\ [(gC^{-1})/(gtx + h)]\, \frac{1}{C} \prod X_{ij}, \tag{3.17}$$

where $D \equiv gt + h$. This term is not divergent for those divergent subgraphs containing t-paths. However, divergences containing no t-paths have to be renormalized by using the above analysis. The only scaling sets which, together with set x, give leading behavior are those T-sets that are logarithmically divergent. If there are n such T-sets consistent with delta function constraints, and if m is the number of distinct divergent subgraphs belonging to these n sets, then the number of scaling sets giving leading behavior is $n + m + 1$. Thus, for example, the last term in I_G^2 for the graph of Fig. 5(a) has a leading behavior of $t^2 \ln {}^4t$.

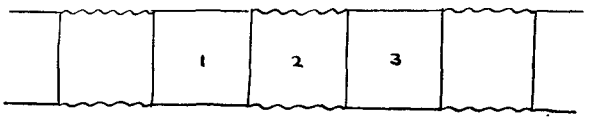


FIG. 6. A two-fermion loop graph.

The fact that in this rule we do not include the divergent subgraphs containing t-paths in calculating m illustrates the proviso we made on the rule stated in Sec. (3B1). If we renormalize for more than one divergent subgraph containing t-paths, the leading behavior of the renormalized term is lowered by at least one power of t. Hence the term with maximum leading behavior is that term where only one divergence containing t-paths is renormalized. Therefore, the leading behavior of the term of I_G^2, where G is the graph of Fig. 6 for which both loops 1 and 3 (and consequently the subgraph consisting of loops 1, 2, 3) are divergent, is only $t^2 \ln {}^3t$. This is, in fact, the leading behavior for the complete Feynman integral, since no other terms in I_G^2 with $t^2 \ln {}^bt (b \geq 0)$ behavior are divergent. This result agrees with the leading behavior for the graph of Fig. 1.

4. SUMMARY

We can summarize our analysis with the following procedure for determining the leading behavior of any Feynman integral $F_{G'}$, where G is a planar graph in the meson–meson scattering process.

(a) If G contains no divergent subgraphs, we simply determine the maximum number of T-sets which can be scaled for any one term of the Chisholm expansion. We can state this differently. If an external meson line to a T-set lies in region $R_1(R_4)$ of the T-set, we will call this meson line a $p_1(p_4)$ meson line. We then look for the maximum number of T-sets, consistent with scaling delta function constraints, and consistent with the fact that two T-sets can possess a $p_1(p_4)$ meson line in common only if a vertex of the meson line is common to both T-sets. For instance, in the example of Fig. 7, delta-

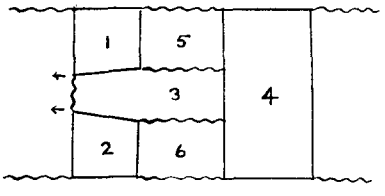


FIG. 7. Conflicting arrow configurations.

function constraints allow us to scale the three T-sets—loops $(1 + 4 + 5)$, loops $(2 + 4 + 6)$, and loop 4. But there are no terms in the Chisholm expansion for which we can scale all three sets. This is simply because for those terms of the Chisholm expansion for which the set consisting of loops $(1 + 4 + 5)$ is a t^2 scaling set, meson line (a) conveys a p_1 momentum from loop 2 to pair with a p_4 momentum in loop 1, whereas for those terms of the Chisholm expansion for which the set consisting of loops $(1 + 4 + 5)$ is a t^2 scaling set, meson line (a) conveys a p_4 momentum from loop 2 to pair with a p_1 momentum in loop 1. The two classes of terms are disjoint. We will call this second constraint on the number of T-sets the constraint of requiring compatible arrow configurations. Let the maximum number of T-sets consistent with delta-function constraints and with compatible arrow configurations be n. The leading behavior is then $t^2 \ln {}^b t$, where $b = \max(1, n)$.

(b) If G contains divergent subgraphs, then we must consider the set of terms of the Chisholm expansion that are divergent for a specific collection (C) of divergent subgraphs that

(i) are cut by t-partitions,
(ii) do not contain t-paths.

We look for that term of the set for which we can scale the maximum number of T-sets. Let this maximum number be n_c, and the number of the divergent subgraphs belonging to the n_c T-sets be m_c.

We then determine the maximum number of divergent T-sets consistent with delta constraints. Let this number be n^1.

Finally, we determine the number of divergent subgraphs belonging to G that

(i) are cut by t-partitions,
(ii) do not contain t-paths.

Let the number be m^1. The leading behavior is then $t^2 \ln {}^b t$, where $b = \max(n^1 + m^1 + 1, n_c + m_c)$.

For any order N, the planar graph with maximum leading behavior is that graph with the maximum number of divergences. To be precise, since all graphs of order N have $(\frac{1}{2}N - 1)$ loops, the maximum number of scaling sets is $(\frac{1}{2}N - 2)$. It is evident that this maximum is only achieved if $\max_c n_c = n^1$ and the graph consists of n divergent one-loop meson–meson scattering graphs with m^1 divergent vertex and self-energy subgraphs such that $n^1 + m^1 = \frac{1}{2}N - 2$. The maximum leading behavior for order N is therefore $t^2 \ln {}^{\frac{1}{2}N-1} t$.

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On an Algebraic Method for the Decomposition of Direct Products of Representations of the Groups $A_2(SU(3))$ and $B_2(SO(5))$

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A prescription for the decomposition of the direct product of two irreducible representations of A_2 and B_2 is given, which is completely general and direct, i.e., it does not make use of any auxiliary means like Young tableau or Cartan–Stiefel diagrams although it is based on the latter. The addition of weights alone under the observation of certain rules gives the desired result. This method can in principle be generalized to the semisimple groups of arbitrary rank provided an algebraic expression for the multiplicities of the weights contained in an irreducible representation can be found.

INTRODUCTION

THIS work is based on the analysis given by Speiser[1] and by Antoine and Speiser[2,3] in lecture notes and two papers, respectively. These publications give, among other things, a graphical method for the decomposition of direct products of two irreducible representations for rank 2 groups. It consists in constructing the weight diagram of one of the two irreducible representations involved and in graphically superimposing this weight diagram onto that point in the two-dimensional Cartan–Stiefel diagram which characterizes the other irreducible representation.[4] But since the dimension of the diagrams equals to the rank of the group this method is limited to rank 2 groups. Due to this situation it might be of interest to write down the corresponding algebraic treatment for rank 2 groups such that the method becomes independent of the explicit construction of the diagrams. This algebraic method might be then not more limited to rank 2 groups but have the property that it can be generalized to groups of arbitrary rank.

In this paper a first step in this direction is done by giving a complete algebraic method for the decomposition of direct products for A_2 and B_2. On the one hand, this method can be generalized in principle to groups of arbitrary rank the only difficulty being to find an algebraic expression for the multiplicity structure of the weights contained in an irreducible representation for the particular group in question.

On the other hand, this method might be useful for the decomposition of direct products in A_2, B_2, and D_2 themselves, in the case when the dimensionality of the two irreducible representations forming the direct product is high and their weight diagrams unknown. In addition this method might be used to find the Clebsch–Gordan series by means of an electronic computer. In this case the method is already completely general, i.e., it works for groups of arbitrary rank since then an algebraic expression for the multiplicities is not necessary.

Section 1 lists briefly some of the results given by Antoine and Speiser. For details the reader is referred to the original papers.[1–3] Section 2 contains the conditions which have to be observed in order that a weight belongs to the Clebsch–Gordan series. Section 3 gives the construction of the weight diagram of an irreducible representation $D(m)$ with highest weight m for A_2, and B_2. Section 4 is a summary. In the Appendix the decomposition of the direct product for A_2 in (p, q) notation is given as an example. This part is insofar self-contained as it gives a working prescription for the decomposition for the group A_2.

1.

Let m and m' be highest weights corresponding to the irreducible representations $D(m)$ and $D(m')$, respectively. Let $X(m' + R_0)$ denote the alternating elementary sum (a.e.s.)[5,6] corresponding to the weight $(m' + R_0)$ and $\chi(m)$ the character of the irrep. $D(m)$. Then from

$$D(m) \otimes D(m') = \sum_{m''} D(m'') \tag{1}$$

the relation

$$\chi(m)X(m' + R_0) = \sum_{m''} X(m'' + R_0) \tag{2}$$

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[1] D. Speiser, *Group Theoretical Concepts and Methods in Elementary Particle Physics* (Gordon and Breach Science Publishers, Inc., New York, 1962).

[2] J. -P. Antoine and D. Speiser, J. Math. Phys. 5, 1226 (1964).

[3] J. -P. Antoine and D. Speiser, J. Math. Phys. 5, 1560 (1964).

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

[5] Also called characteristic.

[6] H. Boerner, *Representations of Groups* (North-Holland Publishing Company, Amsterdam, 1963), Chap. 7.

can be obtained (see Ref. 1). Equation (2) expresses the fact that by adding the weight diagram of the irreducible representation $D(m)$ [i.e., the exponents of $\chi(m)$] to the exponents of the a.e.s. $X(m' + R_0)$ all a.e. sums $X(m'' + R_0)$ are obtained which correspond to the highest weights m'' in the decomposition of the direct product of the two irreducible representations $D(m)$ and $D(m')$. If only the term corresponding to the dominant weight (d.w.) in $X(m' + R_0)$ is taken into account, then (2) says that by adding the weight diagram of $D(m)$ to $(m' + R_0)$ the m'' in the resulting weights $(m'' + R_0)$ are the highest weights of the irreducible representations in the decomposition of $D(m) \otimes D(m')$ if

(I) all m'' are omitted whose a.e.s. is equal to zero, i.e., the m'' which lie on a singular hyperplane[6] and

(II) each pair of weights is omitted whose a.e. sums differ in sign only, i.e., each pair of weights which differs by a reflection $S \in W$ only,[6] W being the Weyl group.

2.

In this section the meaning of the conditions (I) and (II) is studied. In order to see this meaning it has to be known what the application of the Weyl group W to a weight m means. This is, however, well known and the application of W to a weight m consists for the A_l groups in all possible permutations of its components; and for the B_l and C_l groups in all possible permutations of its components together with all possible changes of sign.

Condition (I): If a weight lies on a singular hyperplane, then there exists at least one $S \in W$ (the reflection on that plane) such that $Sm = m$, i.e., that m is left unchanged by S. Knowing how the Weyl group operates on a weight it is clear that such a weight has at least two equal components for A_l; and at least two components m_i, m_j such that $m_i = \pm m_j$ or at least one component $m_k = 0$ for B_l and C_l.

Condition (II): If a pair of weights is such that their a.e. sums differ in the sign only, then they go over into each other by a reflection $S \in W$. Therefore, for A_l such a pair of weights differs by an odd permutation of its components, and for B_l and C_l such a pair of weights differs by an odd permutation with or without a change of sign of the two permuted components or this pair differs simply by having a different sign for one component.

3.

Let m be a highest weight. The weight diagram of the irreducible representation $D(m)$ is constructed now.

Since it is known how the Weyl group W operates on a weight, only the dominant weights $m^{(d)}$ and their multiplicity d have to be found. The whole weight diagram is given by applying W onto them. Equation (2) can therefore be read as [considering the $S = 1$ term of $X(m' + R_0)$ only]

$$\{de^{iSm^{(d)}}\} \cdot e^{i(m'+R_0)} \supseteq \{e^{i(m''+R_0)}\}, \qquad (3)$$

S ranges over W,

where after applying conditions (I) and (II) the equality sign holds. The dominant weights can be found easily. For a given highest weight m they are obtained from the relation

$$m + k_1\beta_1 + \cdots + k_l\beta_l, \qquad k_i \text{ nonnegative integers}, \qquad (4)$$

$-\beta_1, -\beta_2, \cdots, -\beta_l$ the primitive roots of the group in question, if only the weights are taken for which the condition holds to be dominant.[3]

In order to find the multiplicity for these dominant weights first the multiplicities of $1/\Delta$, $\Delta = X(R_0)$, are calculated by using the expression derived for it by Antoine and Speiser.[2] Then from $\chi(m) = X(m + R_0)/\Delta$ the multiplicities of the dominant weights will be derived.

Now, $1/\Delta$ can be written [Ref. 2, (17)] as

$$1/\Delta = \sum_{k_1=0}^{\infty} \sum_{k_2=0}^{\infty} \cdots \sum_{k_n=0}^{\infty} \exp\left[i\left(\sum_{j=1}^{n} k_j\beta_j - R_0, \varphi\right)\right], \qquad (5)$$

the k_i being nonnegative integers, the β_i *all* the negative roots. The multiplicity of a particular vector of $1/\Delta$, let's say γ, is then given by the number of ways γ can be written as a sum over *all* n negative roots with different nonnegative integers k_i as

$$\gamma = k_1\beta_1 + \cdots + k_l\beta_l + \cdots + k_n\beta_n - R_0, \qquad l \leq n. \qquad (6)$$

The multiplicities of the dominant weights can be obtained from [Ref. 2, (19)]

$$\chi = \sum_{k_1=0}^{\infty} \cdots \sum_{k_n=0}^{\infty} \sum_{S \in W} \delta_s \times \exp\left\{i\left[\sum_{j=1}^{n} k_j\beta_j + S(m + R_0) - R_0, \varphi\right]\right\} \qquad (7)$$

as the number of times a dominant weight M can be written as

$$M = k_1\beta_1 + \cdots + k_l\beta_l + \cdots + k_n\beta_n + S(m + R_0) - R_0 \qquad (8)$$

with different nonnegative integers k_i for every $S \in W$. If $S \in W$ is not a reflection, this number is counted positive; if $S \in W$ is a reflection, this number is counted negative. But from (8) it is easy to see that for every given $S \in W$ the number of times M can be written with different coefficients k_i just equals to the multiplicity of the vector

$$\gamma = M - S(m + R_0) = k_1'\beta_1 + \cdots + k_l'\beta_l - R_0 \qquad (9)$$

of $1/\Delta$. Therefore only the multiplicity structure of $1/\Delta$ has to be known, then the multiplicity of a dominant weight can be calculated automatically.

While up to this point the considerations are general, the rest of the paper is restricted to A_2 and B_2(D_2 as the direct product $A_1 \otimes A_1$ is trivial). This is due to the lack of knowledge of algebraic expressions for the multiplicity structure of the dominant weights for the other groups. But doubtless, such algebraic expressions can be found for other groups too.

For A_2 all dominant weights $m^{(d)}$ corresponding to an irreducible representation with highest weight m are obtained from the relation

$$m^{(d)} = m + r\beta_1 + t\beta_2 \qquad (10)$$

(r, t nonnegative integers, $-\beta_1$, $-\beta_2$ the primitive roots), if r and t are varied and all weights collected for which $m_1 \geq m_2 \geq m_3$ holds (i.e., the condition for a weight to be dominant). The multiplicity for some given vector $\gamma = r\beta_1 + s\beta_2 - R_0$ of $1/\Delta$ is given by the number of ways γ can be written as

$$\gamma = a\beta_1 + b\beta_2 + c(\beta_1 + \beta_2) - R_0, \qquad (11)$$

a, b, c nonnegative integers.

Therefore for given r and t the multiplicity of $1/\Delta$ is

$$\begin{matrix} r + 1, & \text{if} \quad t \geq r, \\ t + 1, & \text{if} \quad r \geq t. \end{matrix} \qquad (12)$$

The multiplicity of a dominant weight M is now calculated by using relation (9). From the properties of the roots it can be seen easily that out of the $S \in W$ only the identity and the two reflections S' and S'' on the planes perpendicular to β_1 and β_2 can contribute to the multiplicity of a dominant weight [for any other $S \in W$ there would be negative r', t' in (9)]. From (10) and (9) therefore follows for $S = 1$

$$r' = r, \qquad t' = t,$$

and for S' and S''

$$\begin{cases} t' = m_2 - m_1 + t - 1, \\ r' = r, \end{cases} \qquad \begin{cases} t' = t, \\ r' = m_3 - m_2 + r - 1, \end{cases}$$

such that the multiplicity of the dominant weight (10) becomes[7]

$$\begin{aligned} &(r + 1)\Theta(t - r) + (t + 1)\Theta(r - t - 1) \\ &\quad - (m_2 - m_1 + t)\Theta(m_2 - m_1 + t - 1) \\ &\quad - (m_3 - m_2 + r)\Theta(m_3 - m_2 + r - 1), \end{aligned} \qquad (13)$$

where

$$\Theta(x) = 1, \quad x \geq 0; \qquad = 0, \quad x < 0.$$

But this is nothing else than the well-known result that the multiplicity of the counters increases by 1 in each step by going from the highest weight along $\beta_1 + \beta_2$ while it becomes constant as soon as the boundary of the fundamental domain is reached (Fig. 1).

For B_2 the dominant weights are obtained from

$$m^{(d)} = m + r\beta_1 + t\beta_2, \qquad r, t \text{ nonnegative integers}, \qquad (14)$$

if again $-\beta_1$ and $-\beta_2$ are the primitive roots and only the weights are taken for which $m_1 \geq m_2 \geq 0$. The multiplicity structure of the dominant weights however is much more complicated then as it is in the other case (Fig. 2). In order to obtain an ex-

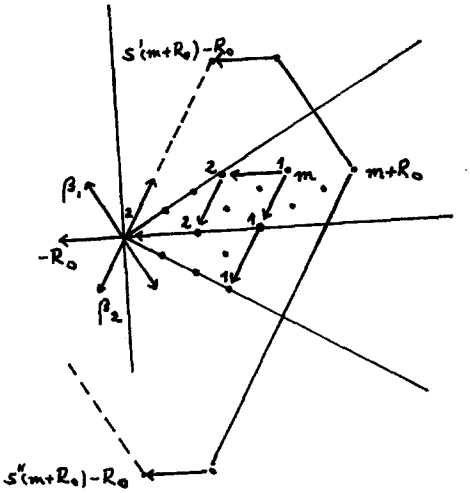

FIG. 1. Weight diagram for A_2. The highest weight of the irreducible representation $\frac{1}{3}(3, -1, -2)$ is denoted by m. The arrows show the way the dominant weights are obtained, the numbers denoting their multiplicity. From $S'(m + R_0) - R_0$ the dominant weight (0, 0, 0) can be obtained in just one way.

[7] Reference 3, Fig. 6, p. 1563.

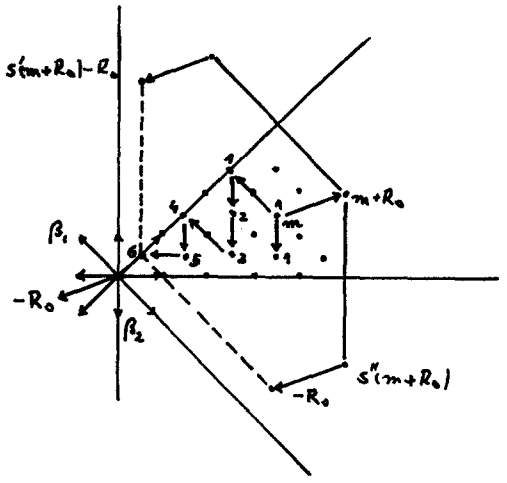

FIG. 2. Weight diagram for B_2. The arrows indicate how the dominant weights of the irreducible representation $m = \frac{1}{2}(7,3)$ are obtained, the numbers denoting their multiplicity. The smallest dominant weight can also be reached from $S'(m + R_0) - R_0$ and $S''(m + R_0) - R_0$ (in a unique way).

pression for the multiplicities of the dominant weights such an expression is found again first for $1/\Delta$. The multiplicity of any vector γ of $1/\Delta$,

$$\gamma = r\beta_1 + t\beta_2 - R_0 \tag{15}$$

is given by the number of ways γ can be written as

$$\gamma = a\beta_1 + b\beta_2 + c(\beta_1 + \beta_2) + d(\beta_1 + 2\beta_2) - R_0, \tag{16}$$

a, b, c, d nonnegative integers,

which is equivalent to all possible ways of expressing r and t as

$$r = a + c + d, \qquad t = b + c + 2d. \tag{17}$$

From this relation the multiplicity of a vector γ with given r and t can be seen to be:

(1) for even t

$$\begin{aligned} &\tfrac{1}{2}(r+1)(r+2), \quad \text{if} \quad t \geq 2r; \\ &i^2 + 2i + 1 + \tfrac{1}{2}(r+1)(r+2) - (i+1)(2i+2), \\ &\quad \text{if} \quad 2r > t > r; \qquad i = r - \tfrac{1}{2}t, \\ &i^2 + 2i + 1, \qquad i = \tfrac{1}{2}t, \quad \text{if} \quad t \leq r. \end{aligned} \tag{18}$$

(2) for odd t

$$\begin{aligned} &\tfrac{1}{2}(r+1)(r+2), \quad \text{if} \quad t \geq 2r; \\ &i(i+1) + \tfrac{1}{2}(r+1)(r+2) - i(2i+1), \\ &\quad \text{if} \quad 2r > t > r; \qquad i = [r - \tfrac{1}{2}(t-1)], \\ &\tfrac{1}{4}(t+1)(t+3), \quad \text{if} \quad t \leq r. \end{aligned} \tag{19}$$

Again, as in the case for A_2 it can easily be seen from the properties of the roots that only the two domains adjacent to the fundamental domain can contribute to the multiplicity of a dominant weight. Since they differ by a reflection from the fundamental domain the multiplicity they contribute is negative. From (9) and (14) then follows for $S = 1$

$$r' = r \quad \text{and} \quad t' = t \tag{20}$$

and for the two reflections S' and S'',

$$\begin{cases} r' = m_2 - m_1 + r - 1, \\ t' = t, \end{cases} \qquad \begin{cases} r' = r, \\ t' = t - (2m_3 + 1), \end{cases} \tag{21}$$

respectively. Thus the multiplicity of a dominant weight (14) is given by (18) and (19) subtracting the values obtained by inserting the nonnegative r', t' of (21).

4.

We can summarize therefore: Given two irreducible representations $D(m)$ and $D(m')$ find the dominant weights $m^{(d)}$ for one of the irreducible representations, say $D(m')$, and their multiplicity d(Sec. 3). Form all weights which can be obtained by the application of the Weyl group (Sec. 2). All these weights form the weight diagram of the irreducible representation $D(m')$. Add all these weights individually to $(m + R_0)$, R_0 being one half of the sum over the positive roots, and select out the weights which have the properties stated in Sec. 2. If from the remaining weights R_0 is subtracted, then all the highest weights in the decomposition of $D(m) \otimes D(m')$ have been obtained.

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I should like to thank Professor B. Vitale and F. Zaccaria for useful discussions.

APPENDIX

As an example, the decomposition is done for $SU(3)$ in the (p_1q) notation, $p = (m_1 - m_2)$, $q = (m_2 - m_3)$. The (p_1q) which correspond to the dominant weights of the irreducible representation (l_1, l_2) and their multiplicity are found in the following way (as can be seen from Sec. 3):

(a) Subtract 2 from one component, add 1 to the other. Continue this way as long as for the resulting (p_1q) holds $p \geq 0$, $q \geq 0$, $q \geq 0$. The d.w.'s corresponding to this set have multiplicity 1.

(b) Subtract 1 from both components of (l_1, l_2) and perform (a). The resulting set has multiplicity 2. Subtract 1 from $(l_1 - 1, l_2 - 1)$ and perform

(a). The resulting set has multiplicity 3. Continue as long as $l_1 - r \geq 0, l_2 - r \geq 0$, r some nonnegative integer. The multiplicity increases by 1 with each step.

(c) From the last set which can be got by (b) take the "second" member, i.e., the one which is obtained from the member $(l_1 - r, l_2 - r)$ of this set by subtracting 2 and adding 1 (there is only one such member) and perform (b). From the resulting set take again the "second" member and perform (b) and so on. The multiplicity does not increase further. (See Fig. 1.)

All the (p, q) which correspond to the weight diagram of (l_1, l_2) are now obtained by applying the Weyl group onto the obtained (p, q). It is easy to verify, that the application of the Weyl group to a (l_1', l_2') results in the set (Sec. 2)

$$\begin{matrix}(l_1', l_2') & (l_2', l_3') & (l_3', l_1') \\ (-l_2', -l_1') & (-l_3', -l_2') & (-l_1', -l_3')\end{matrix}, \quad l_3 = -(l_1 + l_2).$$

These (p, q) have now to be added individually to $(l_1 + 1, l_2 + 1)$. To the resulting set the conditions (I) and (II) have to be applied, which are easily seen to be (Sec. 2):

(I) cancel every (p, q) for which

$$l_1 = 0 \quad \text{or} \quad l_2 = 0 \quad \text{or} \quad l_1 = -l_2;$$

(II) if there occurs a p or a q with a negative sign, the (p, q) will be of the form $(-l_2, -l_1)$ or $(-l_1, l_1 + l_2)$ or $(l_1 + l_2, -l_2)$. Find the corresponding (l_1, l_2) and cancel both.

The only thing left is to subtract $(-1, -1)$ from the remaining set in order to obtain the Clebsch–Gordan series.

For the particular values (5, 2) and (4, 1) this looks as follows. The dominant weights and their multiplicities are

$$\begin{array}{lll} (4,1) \xrightarrow{(a)} (2,2) \xrightarrow{(a)} (0,3) & & d = 1 \\ \quad\downarrow (b) & & \\ (3,0) \xrightarrow{(a)} (1,1) & & d = 2 \\ \qquad\qquad\downarrow (c) & & \\ \qquad\quad (0,0) & & d = 2 \end{array}$$

The sets of equivalent weights with $d = 1$ added to (6, 3) are

(10, 4) (7, −2) (1, 7) (5, −1) (11, 2) (2, 8);

(8, 5) (8, −1) (2, 5) (4, 1) (10, 1) (4, 7);

(6, 6) (3, 3) (9, 0);

and the sets of equivalent weights with $d = 2$ added to (6, 3) are

(9, 3) (6, 0) (3, 6); (7, 4) (7, 1) (4, 4); (6, 3)
(5, 2) (8, 2) (5, 5).

Now, (9, 0) and (6, 0) have to be canceled [condition (I)]. (5, −1) cancels with (4, 1), (7, −2) with one of the (5, 2) and (8, −1) with one of the (7, 1) [condition (II)]. Thus

$$\begin{aligned}(5,2) \otimes (4,1) = {} & (9,3) + (10,1) + (0,6) \\ & + (1,7) + (7,4) + (9.0) + (1,4) + (3,6) \\ & + (5,5) + (2,2) + (8,2) + (8,2) + (2,5) \\ & + (2,5) + (6,3) + (6,3) + (4,1) + (6,0) \\ & + (7,1) + (7,1) + (3,3) + (3,3) + (4,4) \\ & + (4,4) + (5,2) + (5,2).\end{aligned}$$

Scattering Cross Section for a Beam of Wave Packets

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The scattering cross section is evaluated for a beam of wave packets of almost arbitrary form. It is found that this cross section is the superposition of the cross sections of various plane waves, which make up the wave packet without interference. For wave packets of well-defined momentum, the usual rule that the scattering cross section is the absolute square of the scattering amplitude is regained.

1. INTRODUCTION

BY a well-known rule, the scattering cross section for a static potential $V(\mathbf{x})$ (which falls off at infinity faster than $1/x$) may be read off the stationary scattered wave. This stationary wave is a solution of the time-independent Schrödinger equation

$$\frac{\hbar^2}{2m}(k^2 + \nabla^2)\psi_{\mathbf{k}}^+(\mathbf{x}) = V(\mathbf{x})\psi_{\mathbf{k}}^+(\mathbf{x}), \qquad (1.1)$$

with asymptotic form (for large x)

$$\psi_{\mathbf{k}}^+(\mathbf{x}) \simeq e^{i\mathbf{k}\cdot\mathbf{x}} + f_{\mathbf{k}}^+(\Omega - \Omega_{\mathbf{k}})(e^{ikx}/x). \qquad (1.2)$$

We use x for $|\mathbf{x}|$, k for $|\mathbf{k}|$; Ω stands for the angles specifying the direction of the vector $\mathbf{x}$, $\Omega_{\mathbf{k}}$ for those specifying the direction of $\mathbf{k}$. The differential cross section for scattering from direction $\Omega_{\mathbf{k}}$ to Ω is then

$$\sigma(\Omega - \Omega_{\mathbf{k}}) = |f_{\mathbf{k}}^+(\Omega - \Omega_{\mathbf{k}})|^2. \qquad (1.3)$$

An elementary approach[1] derives (1.3) by describing the incident beam by a plane wave, the static situation in which the beam is on by stationary scattering waves $\psi_{\mathbf{k}}^+(\mathbf{x})$. When the outgoing flux described by the scattered part of (1.2) is compared to the plane wave part of the same wave function, Eq. (1.3) follows. A more elaborate treatment (of Chew and Low[2]) considers a beam of wave packets, and shows that Eq. (1.3) is in fact justified, provided that certain conditions on the wave packets are satisfied. These conditions require that the wave packets be well defined in momentum, and be broader in space than the range of the potential.

In this paper, we evaluate exactly the cross section for scattering of a beam of wave packets with almost no assumptions on their form. This is not difficult, and the result is surprisingly simple: it is equivalent to the superposition of the cross sections of the various plane waves involved in the wave packet *without any interference*. For wave packets sharply defined in momentum, Eq. (1.3) is regained.

The wave packet is assumed to contain only motion towards the target and no motion away from the target. More precisely, if the wave packet is described in the space of wave vectors by a function $\phi(\mathbf{k})$ [see Eqs. (2.1)–(2.3) below], the following is satisfied: A "median direction of motion of the wave packet" may be chosen with the criterion that every wave vector $\mathbf{k}$ within the support of $\phi(\mathbf{k})$ deviates from this direction by an angle not larger than $\frac{1}{2}\pi$. Apart from this (and normalization), $\phi(\mathbf{k})$ is arbitrary.

2. SCATTERING OF A SINGLE WAVE PACKET

Consider a wave packet

$$\Phi(\mathbf{x}, t) = \int \frac{d^3\mathbf{k}}{(2\pi)^{\frac{3}{2}}}\phi(\mathbf{k}) \exp i[\mathbf{k}\cdot\mathbf{x} - (\hbar k^2/2m)t] \qquad (2.1)$$

with

$$\int |\phi(\mathbf{k})|^2 d^3\mathbf{k} = 1. \qquad (2.2)$$

$\Phi(\mathbf{x}, t)$ describes the motion of one free particle and is properly normalized for all t:

$$\int |\Phi(\mathbf{x}, t)|^2 d^3\mathbf{x} = 1. \qquad (2.3)$$

A wave packet, which describes the motion of a particle influenced by the potential $V(\mathbf{x})$, but becomes identical to (2.1) asymptotically for large negative time is,

$$\Psi(\mathbf{x}, t) = \int \frac{d^3\mathbf{k}}{(2\pi)^{\frac{3}{2}}}\phi(\mathbf{k})\psi_{\mathbf{k}}^+(\mathbf{x}) \exp[-i(\hbar k^2/2m)t]. \qquad (2.4)$$

This is the wave packet which "describes the scattering of the wave packet (2.1) from the potential $V(\mathbf{x})$."

We now evaluate the probability that a particle

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[1] A. Messiah, *Mecanique Quantique* (Dunod Cie., Paris, 1959), Tome I, Chap. X, Sec. 3, pp. 315–316 [English transl.: John Wiley & Sons, Inc., New York (1961), Vol. 1, pp. 371–2].

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described by Eq. (2.4) will be detected by a counter situated at a distance R from the origin, and blocks a solid angle Γ. This is the same as the probability for a particle to be found in a cone of solid angle Γ (with vertex at the origin) and at a distance greater than R from the origin. This probability is

$$P(\Gamma) = \lim_{t\to\infty} \int_R^\infty x^2\, dx \int_\Gamma d\Omega\, |\Psi(\mathbf{x}, t)|^2. \tag{2.5}$$

The counter is situated far enough from the center of the potential to be considered in the asymptotic region. This is always so in practice, and it is necessary if a theory of scattering depending on angles only is desired. Equation (2.5) involves $\Psi(\mathbf{x}, t)$ only at distances greater than R, so that the asymptotic form of $\Psi(\mathbf{x}, t)$ may be used. This means that the asymptotic form of $\psi_{\mathbf{k}}^+(\mathbf{x})$, Eq. (1.2), may be substituted in Eq. (2.4). Before the substitution, it is convenient to replace the plane wave in Eq. (1.2) by its asymptotic form in spherical coordinates:

$$e^{i\mathbf{k}\cdot\mathbf{x}} \simeq (2\pi/ikx)(\delta(\Omega - \Omega_{\mathbf{k}})e^{ikx} - \delta(\Omega + \Omega_{\mathbf{k}})e^{-ikx}). \tag{2.6}$$

With these substitutions Eq. (2.4) becomes

$$\Psi(\mathbf{x}, t) \simeq \int \frac{d^3\mathbf{k}}{(2\pi)^{\frac{3}{2}}}\, \phi(\mathbf{k}) \exp\left[- i(\hbar^2k^2/2m)\, t\right] \times [(e^{ikx}/x)g^+(\Omega - \Omega_{\mathbf{k}}) - (e^{-ikx}/x)g^-(\Omega + \Omega_{\mathbf{k}})], \tag{2.7}$$

where

$$g^+(\Omega) \equiv (2\pi/ik)\ \delta(\Omega) + f_{\mathbf{k}}^+(\Omega), \tag{2.8}$$

$$g^-(\Omega) \equiv (2\pi/ik)\ \delta(\Omega). \tag{2.9}$$

The probability of Eq. (2.5) is evaluated in the limit of positive infinite time. In that limit, only outgoing waves can contribute to $\Psi(\mathbf{x}, t)$; the term containing g^- may be neglected. Thus the desired probability finally becomes

$$P(\Gamma) = \lim_{t\to\infty} \int_R^\infty x^2\, dx \int_\Gamma d\Omega \times \left| \int \frac{d^3\mathbf{k}}{(2\pi)^{\frac{3}{2}}}\, \phi(\mathbf{k}) g^+(\Omega - \Omega_{\mathbf{k}})\, \frac{1}{x} \times \exp i[kx - (\hbar k^2/2m)t] \right|^2 \tag{2.10}$$

$$= \lim_{t\to\infty} \int_R^\infty dx \int_\Gamma d\Omega \int \frac{d^3\mathbf{k}}{(2\pi)^{\frac{3}{2}}} \int \frac{d^3\mathbf{k}'}{(2\pi)^{\frac{3}{2}}}\, \phi(\mathbf{k})\phi^*(\mathbf{k}') \times \exp\{i[(k - k')x - (k^2 - k'^2)(\hbar t/2m)]\} \times g^+(\Omega - \Omega_{\mathbf{k}})[g^+(\Omega - \Omega_{\mathbf{k}'})]^*.$$

As t becomes greater and greater, the exponential in Eq. (2.10) oscillates faster and faster as a function of k and k'. Eventually, it oscillates faster than any oscillation in the functions $\phi^*(\mathbf{k}')$ and $\phi(\mathbf{k})$, which are independent of x and t. At this stage it becomes permissible to evaluate the k and k' integrals in Eq. (2.10) by the "method of the stationary point". This method may be summarized by the formula

$$\int a(q) \exp[ib(q)]\, dq \simeq \exp[\pm\tfrac{1}{4}i\pi](2\pi/|b''(q_0)|)^{\frac{1}{2}} a(q_0) \exp[ib(q_0)], \tag{2.11}$$

where primes denote derivatives with respect to q, q_0 is the stationary point satisfying $b'(q_0) = 0$ (we assume a unique stationary point), and the $\pm$ sign is the same as the sign $b''(q_0)$. Eq. (2.11) is an approximation which becomes better when the oscillation of $\exp[ib(q)]$ becomes faster compared to any oscillations in $a(q)$. When this formula is applied in the limit of infinitely fast oscillation of the exponential, the results obtained are exact.

When (2.11) is applied to the k and k' integrations of (2.10), the stationary points are

$$k_0 = k_0' = (1/\hbar)m(x/t), \tag{2.12}$$

and the probability becomes

$$P(\Gamma) = \lim_{t\to\infty} \int_R^\infty dx \int_\Gamma d\Omega \int d\Omega_{\mathbf{k}} \int d\Omega_{\mathbf{k}'}\, \frac{2\pi m}{\hbar t}\, \frac{1}{(2\pi)^3} \times \left(\frac{1}{\hbar}\, m\, \frac{x}{t}\right)^4 \phi(k_0, \Omega_{\mathbf{k}})\phi^*(k_0, \Omega_{\mathbf{k}'}) \times g^+(\Omega - \Omega_{\mathbf{k}})[g^+(\Omega - \Omega_{\mathbf{k}'})]^*; \tag{2.13}$$

$\phi(\mathbf{k})$ is expressed in polar coordinates as $\phi(k, \Omega_{\mathbf{k}})$. In place of x, it is convenient to adopt k_0 of Eq. (2.12) as a new variable of integration. This turns Eq. (2.13) into

$$P(\Gamma) = \lim_{t\to\infty} \frac{1}{(2\pi)^2} \int_{\hbar m(R/t)}^\infty dk_0 \int d\Omega \int d\Omega_{\mathbf{k}} \int d\Omega_{\mathbf{k}'}\, k_0^4 \times \phi(k_0, \Omega_{\mathbf{k}})\phi^*(k_0, \Omega_{\mathbf{k}'})g^+(\Omega - \Omega_{\mathbf{k}})[g^+(\Omega - \Omega_{\mathbf{k}'})]^*. \tag{2.14}$$

The above expression depends on R and t only in the lower limit of the k_0 integration. In the limit $t \to \infty$, this lower limit becomes 0 and independent of R. We may now choose R large enough to justify the use of the asymptotic form of $\Psi(\mathbf{x}, t)$. The order of limits used here is essential. One may place the counter as far as one pleases, but, once it is placed, one must wait for the particle to reach and pass it; a counter, moving at the same time as the particle, may outrun its quarry.

3. SCATTERING OF A BEAM OF WAVE PACKETS

The flux of a beam is defined as the number of particles crossing a unit area perpendicular to the direction of motion per unit time. For a beam of wave packets there is no unique direction of motion, all motions corresponding to all wave vectors in the support of $\phi(\mathbf{x})$ are possible. We therefore arbitrarily choose some median direction to define the flux. The only property required of this direction is that no wave vector within the support of $\phi(\mathbf{k})$ deviate from it by more than $\frac{1}{2}\pi$. That such a choice is possible is the only limitation on the form of the wave packet (see the end of Sec. 1). The scattering cross section for a solid angle Γ is defined as the ratio of the number of particles detected in the solid angle Γ per unit of time to the flux of the beam. One always assumes that the various particles in the beam are far apart, and that their mutual interaction may be neglected. Under these circumstances, the time cancels out between the definitions of the scattering cross section and the flux. One may simply consider an ensemble of scattering experiments which differ from each other only in that the wave packets are displaced relative to each other in a direction perpendicular to the chosen-median direction of motion. The ensemble is arranged so that in a plane perpendicular to the chosen-median direction, the density of wave packets be one per unit of area. With this normalization, the total number of counts in the solid angle Γ equals the cross section $\sigma(\Gamma)$ for scattering into that solid angle. (The above considerations concern a uniform beam with unlimited lateral extension. See Sec. 4 for a remark on beams with finite width and given cross section.

The displacement of the wave packet of Eq. (2.1) by a space vector $\mathbf{b}$ amounts to replacing $\phi(\mathbf{k})$ by $\phi(k)\exp[i\mathbf{k}\cdot\mathbf{b}]$. With this replacement, all one has to do to obtain the scattering cross section $\sigma(\Gamma)$, is to integrate $P(\Gamma)d^2\mathbf{b}$, the $d^2\mathbf{b}$ integration ranges over a plane perpendicular to the chosen-median direction of motion. We choose our z-axis along the median direction of motion, so that $d^2\mathbf{b} = db_x db_y$.

At this stage it is convenient to rewrite Eq. (2.14) in terms of two integrations on three-dimensional vectors $\mathbf{k} = (k, \Omega_\mathbf{k})$ and $\mathbf{k}' = (k', \Omega_{\mathbf{k}'})$

$$P(\Gamma) = \frac{1}{(2\pi)^2}\int_\Gamma d\Omega \int d^3\mathbf{k} \int d^3\mathbf{k}'\ \delta(k-k')\phi(\mathbf{k})\phi^*(\mathbf{k}') \times g^+(\Omega-\Omega_\mathbf{k})[g^+(\Omega-\Omega_{\mathbf{k}'})]^*, \tag{3.1}$$

k and k' have taken the place of k_0 in Eq. (2.14); they are kept equal by the δ-function defined for variables between 0 and ∞. When, in the last expression, we replace $\phi(\mathbf{k})$ by $\phi(\mathbf{k})\exp i\mathbf{k}\cdot\mathbf{b}$ and integrate $db_x db_y$, we find

$$\begin{aligned}\sigma(\Gamma) &= \frac{1}{(2\pi)^2}\int_\Gamma d\Omega \int d^3\mathbf{k} \int d^3\mathbf{k}'\ \delta(k-k')\phi(\mathbf{k})\phi^*(\mathbf{k}') \times g^+(\Omega-\Omega_\mathbf{k})[g^+(\Omega-\Omega_{\mathbf{k}'})]^* \\ &\quad\times \int db_x\, db_y \exp i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{b} \\ &= \int_\Gamma d\Omega \int d^3\mathbf{k} \int d^3\mathbf{k}'\ \phi(\mathbf{k})\phi^*(\mathbf{k}') \\ &\quad\times g^+(\Omega-\Omega_\mathbf{k})[g^+(\Omega-\Omega_{\mathbf{k}'})]^* \\ &\quad\times \delta(k-k')\ \delta(k_x-k_x')\ \delta(k_y-k_y').\end{aligned} \tag{3.2}$$

Now,

$$\begin{aligned}&\delta(k-k')\ \delta(k_x-k_x')\ \delta(k_y-k_y') \\ &= \delta[(k_x^2+k_y^2+k_z^2)^{\frac{1}{2}} - (k_x'^2+k_y'^2+k_z'^2)^{\frac{1}{2}}] \\ &\quad\times \delta(k_x-k_x')\ \delta(k_y-k_y') \\ &= [(k_x^2+k_y^2+k_x^2)^{\frac{1}{2}}/k_z]\ \delta(k_z-k_z')\ \delta(k_x-k_x')\ \delta(k_y-k_y') \\ &= \delta^3(\mathbf{k}-\mathbf{k}')/\cos\theta.\end{aligned} \tag{3.3}$$

Strictly speaking, there ought to be an extra term in the last expression as a result from a possible coincidence of k and k' when $k_x = k_x'$, $k_y = k_y'$, and $k_z = -k_z'$. We neglect this term, because, by our assumptions, the support of $\phi(\mathbf{k})$ lies entirely in the halfspace of positive k_z. The angle θ in Eq. (3.3) is the angle between the vector $\mathbf{k}$ and the z-axis which has been assigned parallel to the chosen-median direction of motion.

Once Eq. (3.3) is substituted in Eq. (3.2), the $\mathbf{k}'$ integration may be performed explicitly so that

$$\sigma(\Gamma) = \int_\Gamma d\Omega \int d^3\mathbf{k}\ |\phi(\mathbf{k})|^2 \times |g^+(\Omega-\Omega_\mathbf{k})|^2 \frac{1}{\cos\theta}. \tag{3.4}$$

$g^+(\Omega-\Omega_\mathbf{k})$ is given by Eq. (2.8). If the solid angle Γ includes directions corresponding to wave vectors within the support of $\phi(\mathbf{k})$, $\sigma(\Gamma)$ becomes infinite. This is because an infinite number of unscattered particles, flow into the solid angle Γ. These cannot be separated from the particles scattered into this solid angle. This effect is well known for forward scattering. With a wave packet, every direction within the support of $\phi(\mathbf{k})$, plays the role of the forward direction. For directions outside the support of $\phi(\mathbf{k})$, however, the δ-function in Eq. (2.8) may be neglected, $g^+(\Omega-\Omega_\mathbf{k})$ may be replaced

by $f_{\mathbf{k}}^{+}(\Omega - \Omega_{\mathbf{k}})$. Therefore, for these directions

$$\sigma(\Gamma) = \int_{\Gamma} d\Omega \int d^3\mathbf{k}\, |\phi(\mathbf{k})|^2 \times |f_{\mathbf{k}}^{+}(\Omega - \Omega_{\mathbf{k}})|^2 \frac{1}{\cos\theta}. \quad (3.5)$$

It is customary to express the cross section $\sigma(\Gamma)$ as an integral over the differential cross section $\sigma(\Omega)$,

$$\sigma(\Gamma) = \int_{\Gamma} d\Omega\, \sigma(\Omega). \quad .6)$$

From Eqs. (3.5) and (3.6), the differential cross section $\sigma(\Omega)$ is identified as

$$\sigma(\Omega) = \int d^3\mathbf{k}\, |\phi(\mathbf{k})|^2\, |f_{\mathbf{k}}^{+}(\Omega - \Omega_{\mathbf{k}})|^2 \frac{1}{\cos\theta}. \quad (3.7)$$

4. CONCLUSION

For a wave packet sharply defined in momentum [so that $f_{\mathbf{k}}^{+}(\Omega - \Omega_{\mathbf{k}})$ is practically constant as a function of $\mathbf{k}$ over the support of $\phi(\mathbf{k})$], one of the mean value theorems may be used to take $|f_{\mathbf{k}}^{+}(\Omega - \Omega_{\mathbf{k}})|^2$ outside the integral in Eq. (3.7). This reduces expression (3.7) to Eq. (1.3), the well-known result for wave packets with well-defined momentum.

For wave packets spread in momentum space, (3.7) is nothing but a superposition of the differential cross sections of the different planewaves in the spectrum of the wave packet *without any interference.* The factor $1/\cos\theta$ may be understood as a renormalization of the flux of the different planewaves. This renormalization is due to the fact that we have defined flux relative to some arbitrarily chosen average direction of motion, while the flux or a planewave is taken relative to the direction of its wave vector $\mathbf{k}$. The angle between the two directions is θ. But, whatever the interpretation of the formula (3.7), it is, as the derivation shows, exact. The only assumption on the form of the wavepacket was that the various directions of motion involved deviate from the median direction by no more than $\frac{1}{2}\pi$.

The same approach could be extended to beams not uniformly extended in space. If these beams have lateral boundaries, or if their flux varies in the plane perpendicular to the median direction of motion, an appropriate weight function must be added to the integration $d^2\mathbf{b}$ in Eq. (3.2).

Linked Cluster Theorem and the Green's Function Equations of Motion for a Many-Fermion System*

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The equations of motion for the general many-time causal Green's functions for a fermion system are iterated and are shown not to lead to unlinked graphs, which is a general proof of the linked cluster theorem. An explicit expression is obtained for the perturbation expansion of an arbitrary Green's functions which is applied to the one- and two-particle Green's functions. By connecting lines systematically in a set of diagrams obtained from the equations of motion, the usual topologically different linked graphs and rules are generated.

I. INTRODUCTION

RECENTLY, some of the dead wood in quantum-electrodynamics has been cleared away by Dirac,[1] using the Heisenberg picture in which the divergent vacuum-to-vacuum graphs do not appear in the theory. The rules for obtaining mathematical contributions from the graphs are the same as the rules obtained in the Schrödinger picture. In the Schrödinger picture the time-development of states is responsible for the vacuum-to-vacuum graphs. In this paper, it will be shown that a similar situation occurs in the many-body problem. The usual method of developing perturbation theory for the Green's functions based on the interaction picture[2] gives vacuum-to-vacuum, or unlinked, graphs. However, by using directly the equations of motion for the Green's functions in the Heisenberg picture, the unlinked terms do not appear. This fact was first shown by Klein and Prange[3] through second order in the one-particle Green's function, but will be proved here to be true in all orders for the general Green's function.

The usual many-body perturbation theory is developed for the Green's functions or propagators by first using the adiabatic theorem[4] to put them in the interaction picture in which they are divided by the ground-state expectation value of the S-matrix. The Green's functions can then be expanded by using Wick's theorem[5] which says that the time-ordered product is equal to the normal-ordered product with all possible pairings. However, some of these pairings lead to unlinked terms. The linked cluster theorem[6] is then proved, which says that the unlinked terms cancel with the expectation value of the S-matrix in the denominator.[7] Then it can finally be stated that the Green's function can be obtained by drawing all topologically different linked graphs, and associating certain factors with each graph. This procedure is given in the upper part of Fig. 1. It has the disadvantage that the unphysical unlinked graphs are introduced as a consequence of Wick's theorem[8] and must be shown to cancel out.

The method which will be developed here is an extension of the work by Klein and Prange[3] on the Green's function equations of motion.[9] The equations of motion for the Green's function can be obtained essentially by differentiating and integrating, making use of the equation of motion for an operator in

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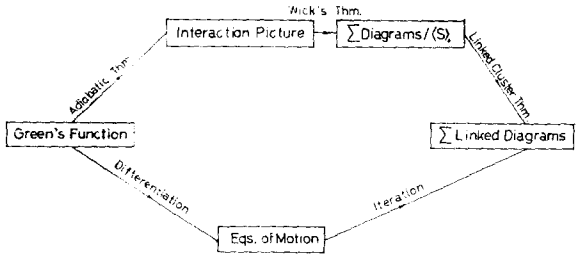


FIG. 1. Alternative methods for developing perturbation theory for the Green's functions. The upper path is the traditional method. The lower path will be discussed in this paper.

the Heisenberg picture, and taking the Fourier transform.[10] The Green's function equations of motion can be solved by iteration which can be shown to lead to perturbation theory in terms of linked graphs only. The unphysical unlinked graphs do not even enter the theory. This procedure is shown in the lower part of Fig. 1.

In the next section, the Green's function equations of motion will be discussed. In Sec. III, the linked cluster theorem will be proved in all generality, and the formal perturbation expansion obtained. In order to illustrate the theory, the one-particle Green's function will be calculated explicitly to third order in Sec. IV. In Sec. V, the two-particle Green's function will be calculated to second order to show that the method is also applicable to higher-particle Green's functions. For the sake of completeness, the derivation of the Green's function equations of motion is given in the Appendix.

II. GREEN'S FUNCTION EQUATIONS

The equations of motion satisfied by the Green's functions or propagators for a many-fermion system have been obtained in a number of papers,[9] but some of the details will be examined here to emphasize the importance of boundary conditions and antisymmetrization. The structure of the equations is essential in proving the linked cluster theorem and in obtaining the rules for constructing the propagators. A complete derivation is given in the Appendix.

The Hamiltonian for a many-fermion system can be written in second quantization as

$$H = \sum_1 e_1 a_1^+ a_1 + \tfrac{1}{4} \sum_{1234} \lambda \langle 12| \ V \ |34\rangle a_1^+ a_2^+ a_3 a_4, \quad (2.1)$$

where the numerals $j = 1, 2, 3, 4$ stand for the momentum $\mathbf{k}_j$ and the spin σ_j (up/down). The kinetic energy of a particle with momentum $\mathbf{k}_1$ is e_1, and the matrix elements of the potential energy V satisfy the following symmetry properties

$$\begin{aligned} \langle 12| \ V \ |34\rangle &= -\langle 12| \ V \ |43\rangle \\ &= -\langle 21| \ V \ |34\rangle = \langle 21| \ V \ |43\rangle. \end{aligned} \quad (2.2)$$

The parameter λ is a strength parameter that can vary between zero and one. The creation operators a_1^+ and the annihilation operators a_1 satisfy the usual fermion anticommutation relations

$$\begin{aligned} [a_1, a_2^+]_+ &= \delta_{12}, \\ [a_1, a_2]_+ &= 0, \\ [a_1^+, a_2^+]_+ &= 0. \end{aligned} \quad (2.3)$$

Instead of solving the Schrödinger equations by using ordinary perturbation theory, we will develop a field-theoretic-type perturbation theory[2] based on the equations of motion[9] satisfied by the Green's functions or propagators of the system.

The general n particle, many-time, causal Green's function for a system with N particles is defined as[11]

$$\begin{aligned} &\mathcal{G}_n(1, 2, \cdots, 2n) \\ &\quad = i\langle N| \ T\{a_1 a_2 \cdots a_n a_{n+1}^+ \cdots a_{2n}^+\} \ |N\rangle, \end{aligned} \quad (2.4)$$

where the expectation value is taken with respect to the exact ground state of the N particle system $|N\rangle$. The annihilation operators and creation operators are all in the Heisenberg picture, which is defined for an arbitrary operator A as

$$A(t) = e^{iHt} A e^{-iHt} \quad (2.5)$$

with a different time associated with each subscript in Eq. (2.4). The time-ordering operator T orders the product of operators with the largest time on the left and the smallest time on the right, in decreasing order, with a plus (minus) sign for an even (odd) permutation of the original order.

An alternative way of writing Eq. (2.4) which is helpful in obtaining the equation of motion is[12]

$$\begin{aligned} &\mathcal{G}_n(1, 2, \cdots, 2n) \\ &\quad = i \sum_P (-1)^P P\langle N| \ A_1 \cdots A_{2n} \ |N\rangle \\ &\qquad \times \theta(1 - 2) \cdots \theta[(2n - 1) - 2n], \end{aligned} \quad (2.6)$$

where the sum is over all permutations P of $2n$ integers, $(-1)^P$ is the sign of the permutation, and

$$A_k = \begin{cases} a_k & \text{if} \quad k \leq n, \\ a_k^+ & \text{if} \quad k > n. \end{cases} \quad (2.7)$$

[10] See, e.g., the procedure used in D. H. Kobe and W. B. Cheston, Ann. Phys. (N. Y.) 20, 279 (1962), to obtain the equations of motion for Bogoliubov quasi-particle propagators.

[11] See, e.g., A. Klein, in *Lectures on the Many-Body Problem*, E. R. Caianiello, Ed. (Academic Press Inc., New York, 1962), p. 279.

[12] V. P. Gachok, Zh. Eksperim. i Teor. Fiz. 40, 879 (1961) [English transl.: Soviet Phys.—JETP 13, 616 (1961)].

The function $\theta(1-2) \equiv \theta(t_1 - t_2)$ is the step function, which is one for positive argument and zero for negative argument. The spectral representation of the many-time causal Green's function[13] can be obtained by taking the Fourier transform of $\mathcal{G}_n$, but this will not be done here.

The equation satisfied by $\mathcal{G}_n$ is usually obtained by differentiating Eq. (2.6) with respect to the time t_1.[11] However, this method singles out a specific time and the equations are not explicitly antisymmetric during the derivation. It also results in an ambiguity concerning the single-particle propagator. A method that eliminates these difficulties is to differentiate and integrate successively.[10] Thus, it can be shown that the operator

$$Z_1 = -ie^{-ie_1t_1}\int_{-\infty}^{\infty} dt_1' \,[(1-c_1)\theta(t_1 - t_1') - c_1\theta(t_1' - t_1)]i\frac{\partial}{\partial t_1'}e^{ie_1t_1'} \tag{2.8}$$

is the unit operator if the boundary condition

$$(1-c_1)[e^{ie_1t_1'}\mathcal{G}_n(1', 2, \cdots 2n)]_{t_1'=-\infty} + c_1[e^{ie_1t_1'}\mathcal{G}_n(1', 2, \cdots 2n)]_{t_1'=\infty} = 0 \tag{2.9}$$

is satisfied. Now, in general, the terms evaluated at plus and minus infinity will be zero in the sense of weak convergence,[14] so that any c_1 would be possible. However, in the case of noninteracting particles, and $n = 1$, we get

$$c_1 = n_1 = \begin{cases} 1 & \text{if} \quad k_1 < k_F, \\ 0 & \text{if} \quad k_1 > k_F, \end{cases} \tag{2.10}$$

where k_F is the Fermi momentum.

If the unit operator Z_1 of Eq. (2.8) is applied to Eq. (2.6) for $\mathcal{G}_n$, the antisymmetrizer applied, and the differentiation is performed using the equation of motion for an operator in the Heisenberg picture, the equation of motion can be obtained in terms of time. Then, if the general Fourier transform operator

$$\mathcal{F}_{2n} = \int_{-\infty}^{\infty} \cdots \int dt_1 \cdots dt_{2n} \exp\left\{i\sum_{j=1}^{2n}\omega_{-j}t_j\right\}, \tag{2.11}$$

where

$$\omega_{-j} = \begin{cases} \omega_j & \text{if} \quad j \leq n, \\ -\omega_j & \text{if} \quad j > n \end{cases} \tag{2.12}$$

is applied, the equation satisfied by the Fourier transform of $\mathcal{G}_n$ is (see the Appendix)

$$\begin{aligned} &G_n(1, 2, \cdots, 2n) \\ &= \mathcal{A}_{1n}\sum{}'(-1)^r G^0(1, 1')h(1'2'3'4') \\ &\quad \times G_{n+1}(3'4'2\cdots n; 2'n+1, \cdots 2n) \\ &\quad - i(-1)^{n-1}\mathcal{A}_{1n}n\mathcal{A}_{n+1,2n}G^0(1, n+1) \\ &\quad \times G_{n-1}(2, \cdots, n; n+2, \cdots 2n). \end{aligned} \tag{2.13}$$

The vertex function is given by[15]

$$h(1234) = (2\pi)^{-3}\tfrac{1}{2}(12|\ V\ |34) \times \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4)\exp(-i\omega_3\epsilon + i\omega_2 2\epsilon). \tag{2.14}$$

The unperturbed single-particle Green's function $G^0(1, 2)$ is defined as

$$G^0(1, 2) = -2\pi\,\delta_{12}\{(1-c_1)/(\omega_1 - e_1 + i0) + c_1/(\omega_1 - e_1 - i0)\}, \tag{2.15}$$

and, in case of no interaction, $c_1 = n_1$ given by Eq. (2.10). The usual form of perturbation theory based on the adiabatic theorem[2] uses $c_1 = n_1$ even in the case of interaction.

If the interaction is spherically symmetric, then this choice of the single-particle propagator is satisfactory.[16] However, if the interaction is not spherically symmetric, the adiabatic theorem is not satisfied[17] and it is necessary to use an unperturbed ground state with the same Fermi surface as the interacting system. A self-consistent potential can be added and subtracted from the Hamiltonian, which changes the single-particle energies so that the unperturbed system has the same Fermi surface.[18] The free-particle propagator[19] appropriate to this unperturbed system can easily be obtained by a modification of the single-particle energy in Eq. (2.8) and the appropriate choice of c_1 in Eq. (2.15), Thus, the formulation here provides a way of transcending the usual difficulties of perturbation theory associated with the adiabatic theorem.

The antisymmetrizer in Eq. (2.13) is defined in the usual way as

$$\mathcal{A}_{1n} = \frac{1}{n!}\sum_P (-1)^P P, \tag{2.16}$$

where P is a permutation of the numbers $1, 2, \cdots, n$, and $(-1)^P$ is the sign of the permutation. The anti-

[13] D. H. Kobe, Ann. Phys. (N. Y.) **19**, 448 (1962).
[14] See, e.g., G. Temple, Proc. Roy. Soc. (London) **A276**, 149 (1963).
[15] The exponential factors in Eq. (2.14) are needed to remove the ambiguity in loop diagrams. They arise naturally in the derivation of the equations of motion given in the Appendix. The limit $\epsilon \to 0+$ is understood in Eq. (2.14).
[16] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).
[17] W. Kohn and J. M. Luttinger, Phys. Rev. **118**, 41 (1960).
[18] A. Klein, Phys. Rev. Letters **4**, 601 (1960).
[19] A. Klein, Phys. Rev. **121**, 950 (1961).

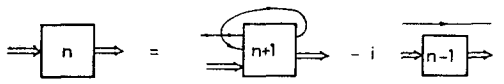


FIG. 2. Graphical representation of the equation of motion for the Green's function G_n.

symmetrizer $\mathcal{A}_{n+1,2n}$ operates on the n variables $n+1, n+2, \cdots, 2n$. The need for the antisymmetrizer in the equations of motion was emphasized in an earlier paper[10] in order to preserve the antisymmetry properties of the original Green's function with respect to interchange of the annihilation operators (or creation operators). It is essential in establishing the connection between the equations of motion method and the usual form of perturbation theory based on Wick's theorem.[2]

Fig. 2 shows the graphical representation of Eq. (2.13) and, for the sake of clarity, is not antisymmetrized. The correspondence between the mathematical quantities and the graphs in Fig. 2 is shown in Fig. 3. In the next section, Eq. (2.13) will be iterated and shown not to lead to unlinked terms.

III. ITERATION OF THE GREEN'S FUNCTION EQUATIONS

The equation of motion for the Fourier transform of the many-time, causal Green's function for an N-particle system obtained in Eq. (2.13) can be written symbolically as

$$G_n = F_n G_{n+1} + J_n G_{n-1}, \tag{3.1}$$

where the operators F_n and J_n are defined by Eq. (2.13). From Fig. 2 it can be seen that the operator F_n acts on a function having $n+1$ lines and connects the top outgoing line with the second incoming line, after crossing the first incoming line. The remaining n incoming lines are then antisymmetrized. The operator J_n adds another line to a function having $n-1$ lines, multiplies by n, and antisymmetrizes both the incoming and outgoing lines.

It will now be shown by induction that G_n satisfies an equation of the type

$$G_n = f_n G_{n+1} + L_n, \tag{3.2}$$

where f_n is a linear operator given by

$$f_n = K_n F_n. \tag{3.3}$$

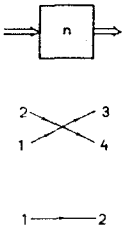


FIG. 3. Correspondence between the graphical quantities of Fig. 2 and the mathematical quantities of Eq. (2.13).

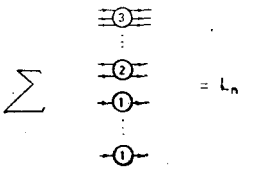


FIG. 4. The linked terms L_n. The number of incoming lines and outgoing lines is n.

The linear operator K_n is not yet specified, but a recursion relation will be found for it. The term L_n is a sum of terms each linked to the outside by n lines, and are either connected or disconnected as shown in Fig. 4. There are no unlinked graphs or ground-state components of the type shown in Fig. 5 that contribute to it.[20] It is assumed to have the form

$$L_n = K_n J_n L_{n-1}, \tag{3.4}$$

where L_{n-1} has a similar definition, J_n is given by Eq. (3.1) and (2.13), and K_n is the as yet unknown operator. However, from Eq. (3.4), it is seen that K_n must not generate unlinked graphs for the assumption to be consistent. Now, we will prove by induction that Eqs. (3.2), (3.3), and (3.4) are indeed valid. In the process we will also discover a recursion relation for K_n.

For $n = 1$ Eq. (3.2) becomes

$$G_1 = f_1 G_2 + L_1. \tag{3.5}$$

However, for $n = 1$, Eq. (3.1) can be written

$$G_1 = F_1 G_2 + J_1 i, \tag{3.6}$$

which is the same form as Eq. (3.5), since $J_1 i$ is a term linked to the outside with no unlinked part. From Eq. (3.3), we have

$$f_1 = K_1 F_1, \tag{3.7}$$

and, from Eq. (3.4), we have

$$L_1 = K_1 J_1 L_0. \tag{3.8}$$

Therefore, by comparing Eqs. (3.5) and (3.6), we have

$$K_1 = 1 \tag{3.9}$$

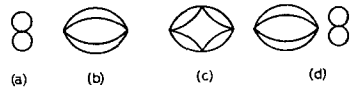


Fig. 5. Examples of unlinked graphs. Graph d is disconnected while the others are connected.

[20] The definitions of linked and unlinked, and connected and disconnected diagrams given here are the same as Nozières (Ref. 2). Linked diagrams are "linked" to the "outside" by external lines, while unlinked diagrams have no external lines. Connected diagrams are those that *cannot* be divided into two or more parts without cutting a line. Diagrams that *can* be so divided are called disconnected.

and

$$L_0 = i. \tag{3.10}$$

The assumption of the form of equations given in Eqs. (3.2), (3.3), and (3.4) is thus consistent for $n = 1$, if the values of K_1 and L_0 in Eqs. (3.9) and (3.10) are used.

The next step in the induction proof is to show that Eqs. (3.2), (3.3), and (3.4) are valid for $n + 1$. For $n + 1$, Eq. (3.1) gives

$$G_{n+1} = F_{n+1}G_{n+2} + J_{n+1}G_n. \tag{3.11}$$

If Eq. (3.2), which is assumed to be true, is substituted into Eq. (3.11), the result is

$$G_{n+1} = F_{n+1}G_{n+2} + J_{n+1}L_n + J_{n+1}f_nG_{n+1}. \tag{3.12}$$

Equation (3.12) can be iterated once to give

$$G_{n+1} = [1 + J_{n+1}f_n][F_{n+1}G_{n+2} + J_{n+1}L_n] + (J_{n+1}f_n)^2G_{n+1}. \tag{3.13}$$

If the equation is iterated an infinite number of times, then the result has the form

$$G_{n+1} = f_{n+1}G_{n+2} + L_{n+1}, \tag{3.14}$$

where

$$f_{n+1} = K_{n+1}F_{n+1} \tag{3.15}$$

and

$$L_{n+1} = K_{n+1}J_{n+1}L_n. \tag{3.16}$$

In order to write Eqs. (3.15) and (3.16) in this form, the function K_{n+1} must be

$$K_{n+1} = \sum_{k=0}^{\infty} (J_{n+1}f_n)^k \equiv [1 - J_{n+1}f_n]^{-1}, \tag{3.17}$$

where the inverse operator is defined by the geometrical series. Since f_n is given by Eq. (3.3), we obtain

$$K_{n+1} = [1 - J_{n+1}K_nF_n]^{-1} \tag{3.18}$$

as a recursion relation that K_n must satisfy in order for Eqs. (3.2), (3.3), and (3.4) to be valid for all integers n. Since the J's and F's are known for all n and Eq. (3.9) shows that $K_1 = 1$, we can obtain all the K's by using Eq. (3.18). If K_n, acting on J_nL_{n-1}, does not generate any ground-state components or unlinked graphs in Eq. (3.4), then K_{n+1} will not generate any unlinked graphs when acting on $J_{n+1}L_n$ because of Eq. (3.18) which relates K_{n+1} and K_n.

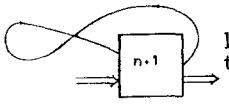


Fig. 6. A graph that would give unlinked terms, but does not contribute to G_n.

Therefore Eq. (3.2) has been established for all integers n by mathematical induction.

Equation (3.2) can itself be iterated by substituting Eq. (3.14) into it for G_{n+1}, and continuing the iteration by using higher-order equations, which gives

$$G_n = \prod_{k=0}^{m-1} f_{n+k}G_{n+m} + \sum_{j=0}^{m-1} \prod_{k=0}^{j-1} f_{n+k}L_{n+j}, \tag{3.19}$$

where the products are to be expanded to the right. The product in the last term is to be taken as unity when $j = 0$. If the limit is now taken as $m \to \infty$, the first term will contain an infinite number of f's and hence V's, so it will not contribute if it is assumed that the perturbation series converges. Hence, the G_n representation

$$G_n = \sum_{j=0}^{\infty} \prod_{k=0}^{j-1} f_{n+k}L_{n+j} \tag{3.20}$$

is obtained. Equation (3.20) still contains L's and f's, but it can be rewritten with the help of Eqs. (3.3) and (3.4) to give

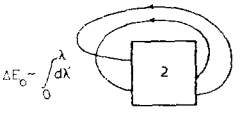
$$G_n = \sum_{j=0}^{\infty} \prod_{k=0}^{j-1} [K_{n+k}F_{n+k}] \times \prod_{l=0}^{n+j-1} [K_{n+j-l}J_{n+j-l}]i. \tag{3.21}$$

Equation (3.21) is the explicit solution for the propagator G_n, since the F's and J's are all known, and the K's can be obtained from Eq. (3.18). Thus, G_n can be evaluated to any finite order in perturbation theory. The unlinked terms of ground-state components, if there are any, must be contained in the G_{n+m} in Eq. (3.19), because the f's, acting on an L, do not produce unlinked terms, since neither the F nor the K produces unlinked terms. Thus, the unlinked terms can only occur in infinite order if the limit $m \to \infty$ is taken, and will be zero if the series converges. Therefore, the n-particle Green's function G_n is just a sum of linked terms, which is a statement of the linked cluster theorem. It has now been proved to all orders for an arbitrary Green's function from the equations of motion.

The reason that the unlinked graphs do not occur in the equations of motion method is that there are no graphs of the type shown in Fig. 6 occurring in Fig. 2. Thus, the allowable ways of connecting the outgoing lines with the incoming lines is restricted in such a way that it is not possible for a ground-state component or unlinked term to be split off. However, in Wick's theorem, all possible pairings are allowed, and some of these cause the unphysical unlinked graphs to appear.

The ground-state energy can be calculated by the equations given by Galitskii and Migdal[9] or by Klein and Prange.[3] The graphical illustration of the ground-state energy is given in Fig. 7. If the expansion for the two-particle Green's function were to be substituted into it, a sum of unlinked connected graphs would be obtained. This statement is sometimes called the linked cluster theorem.[6] However, it follows as a corollary of the more general theorem proved above.[21]

FIG. 7. The shift in the ground-state energy.



IV. SINGLE-PARTICLE PROPAGATOR

In order to illustrate the previous formalism, the single-particle propagator will be calculated to third order. Because of the Dyson equation, the self-energy can also be obtained to the same order by considering just the irreducible self-energy diagrams (contributions to the single-particle propagator that cannot be divided into two parts by cutting just one line).

The traditional approach based on Wick's theorem involves drawing all topologically different graphs, and associating certain factors with each graph. In theory, this approach has reduced the problem as far as possible, but, in practice, it is difficult to draw all topologically different graphs and associate the proper factors with each, especially in a high order. The approach here, while giving the same result, presents a way of generating all the topologically different graphs with the correct factors.

To calculate G_1 we can use Eq. (3.21)

$$G_1 = \sum_{j=0}^{\infty} \prod_{k=0}^{j-1} [K_{k+1}F_{k+1}] \prod_{l=0}^{j} [K_{1+j-l}J_{1+j-l}]i. \quad (4.1)$$

This expression can be expanded, and the first several terms are

$$\begin{aligned} G_1 = {} & iJ_1 + iF_1K_2J_2J_1 \\ & + iF_1K_2F_2K_3J_3K_2J_2J_1 \\ & + iF_1K_2F_2K_3F_3K_4J_4K_3J_3K_2J_2J_1 \\ & + iF_1K_2F_2K_3F_3K_4F_4K_5J_5K_4J_4K_3J_3K_2J_2J_1 + \cdots , \end{aligned} \quad (4.2)$$

where use has already been made of Eq. (3.9) for K_1. In Eq. (4.2), the functions K_2, K_3, K_4, $\cdots$ occur, and are given by Eq. (3.18) as

$$\begin{aligned} K_1 &= 1, && \text{(a)} \\ K_2 &= 1 + J_2F_1 + J_2F_1J_2F_1 \\ &\quad + J_2F_1J_2F_1J_2F_1 + \cdots , && \text{(b)} \\ K_3 &= 1 + J_3K_2F_2 \\ &\quad + J_3K_2F_2J_3K_2F_2 + \cdots , && \text{(c)} \\ K_4 &= 1 + J_4K_3F_3 + \cdots . && \text{(d)} \end{aligned} \quad (4.3)$$

Substituting Eq. (4.3) into Eq. (4.2), grouping terms according to order, and considering terms through fourth order, we obtain

$$\begin{aligned} G_1 = {} & G^0 && (0) \\ & + iF_1J_2J_1 && (1) \\ & + i\{F_1F_2J_3J_2J_1 && (2a) \\ & \quad + F_1J_2F_1J_2J_1\} && (2b) \\ & + i\{F_1F_2F_3J_4J_3J_2J_1 && (3a) \\ & \quad + F_1F_2J_3F_2J_3J_2J_1 && (3b) \\ & \quad + F_1J_2F_1F_2J_3J_2J_1 && (3c) \\ & \quad + F_1J_2F_1J_2F_1J_2J_1 && (3d) \\ & \quad + F_1F_2J_3J_2F_1J_2J_1\} && (3e) \\ & + i\{F_1F_2F_3F_4J_5J_4J_3J_2J_1 && (4a) \\ & \quad + F_1F_2F_3J_4J_3J_2F_1J_2J_1 && (4b) \\ & \quad + F_1F_2F_3J_4J_3F_2J_3J_2J_1 && (4c) \\ & \quad + F_1F_2F_3J_4F_3J_4J_3J_2J_1 && (4d) \\ & \quad + F_1F_2J_3F_2F_3J_4J_3J_2J_1 && (4e) \\ & \quad + F_1J_2F_1F_2F_3J_4J_3J_2J_1 && (4f) \\ & \quad + F_1F_2J_3F_2J_3J_2F_1J_2J_1 && (4g) \\ & \quad + F_1J_2F_1F_2J_3J_2F_1J_2J_1 && (4h) \\ & \quad + F_1J_2F_1F_2J_3F_2J_3J_2J_1 && (4i) \\ & \quad + F_1F_2J_3J_2F_1F_2J_3J_2J_1 && (4j) \\ & \quad + F_1F_2J_3J_2F_1J_2F_1J_2J_1 && (4k) \\ & \quad + F_1F_2J_3F_2J_3F_2J_3J_2J_1 && (4l) \\ & \quad + F_1J_2F_1J_2F_1F_2J_3J_2J_1 && (4m) \\ & \quad + F_1J_2F_1J_2F_1J_2F_1J_2J_1\} && (4n) \\ & + \cdots . && (4.4) \end{aligned}$$

[21] There have been many treatments of the linked cluster theorem from other points of view and in other contexts. A good review of the linked cluster theorem has been given by B. H. Brandow (unpublished). For other references to the subject see C. Bloch and C. De Dominicis, Nucl. Phys. 7, 459 (1958); F. Coester, *ibid.* 7, 421 (1958); C. Bloch and J. Horowitz, *ibid.* 8, 91 (1958); T. Morita, Progr. Theoret. Phys. (Kyoto) 29, 351 (1963); and H. Kümmel, in *Lectures on the Many-Body Problem*, E. R. Caianiello, Ed. (Academic Press Inc., New York, 1962), p. 265.

Equation (4.4) can be written in a more concise way

$$G_1 = G^0 + iF_1 \sum_{n=0}^{\infty} [\text{distinct permutations of } nF\text{'s and } nJ\text{'s}]J_2J_1. \quad (4.5)$$

After the distinct permutations have been made, it is necessary to add subscripts indicating the number of outgoing lines after the application of the operator F or J. The number of outgoing lines or incoming lines in intermediate steps must always be one or more, otherwise the term is zero. For example, in third order, a term of the type

$$FFJFJJJ = F_1F_2J_3F_2J_3J_2J_1 \quad (4.6)$$

is a contribution, but not a term of the type

$$FJJFFJJ = F_1J_2J_1F_0F_1J_2J_1 = 0, \quad (4.7)$$

because F_0 must be zero. Thus, all the terms in Eq. (4.5) with nonpositive subscripts, e.g., F_0, J_0, F_{-1}, J_{-1}, $\cdots$ must be zero.

After the subscripts have been added in Eq. (4.5), the terms remaining are those that come from the expansion of Eq. (4.2). An arbitrary term from Eq. (4.5) can be classified according to the order p and the highest value of the subscript on F, say k. This term would then come from the term with the basic structure $F_1 \cdots F_k J_{k+1} \cdots J_1$ in Eq. (4.2) since, if an F_k exists, there must be $k+1$ lines on which it can act. Since the term is a contribution to G_1, the number of lines must be decreased until there is only one. In Eq. (4.2), there are the appropriate K's inserted between all of the operators. Because of the recursion relation in Eq. (3.18), we can iterate it and obtain

$$K_n = \sum_{\alpha} (J_n \sum_{\beta} \{J_{n-1} \sum_{\gamma} [J_{n-2} \sum_{\delta} (J_{n-3}K_{n-4}F_{n-4})^{\delta}F_{n-3}]^{\gamma}F_{n-2}\}^{\beta}F_{n-1})^{\alpha}, \quad (4.8)$$

where the Greek letters are integers going from zero to infinity. Because of Eq. (4.8), there can be insertions between the operators of the basic structure of the type

$$\{J[J(J \cdots F) \cdots (J \cdots F)F] \cdots \times [J \cdots F]F\}\{J \cdots F\} \cdots \{J \cdots F\}, \quad (4.9)$$

where the number of J's and F's is the same within parentheses. The dots in Eq. (4.9) represent possible insertions of the same kind. The only restriction on the insertions is that the subscripts must be positive and the total number of F's in the term must be p. Any arbitrary term from Eq. (4.5) in pth-order has p F's and $(p+1)$ J's. In the basic structure, there are k F's and $(k+1)$ J's, so there are $(p-k)$ F's and the same number of J's which can be distributed between the operators in the basic structure. In order for k to be the maximum subscript on F, these $(p-k)$ F's and J's must be distributed in the way shown in Eq. (4.9). Conversely, an arbitrary term in the expanded form of Eq. (4.2) corresponds

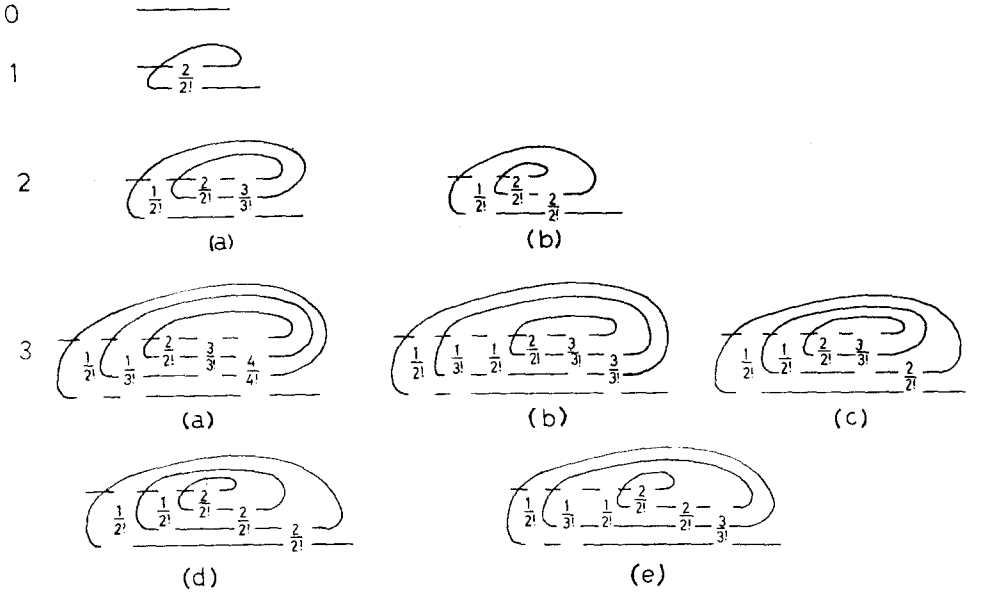


FIG. 8. Diagrams for the single-particle propagator obtained from the Green's function equations of motion.

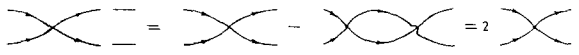


FIG. 9. Equivalence of the lines leaving a vertex.

to a definite contribution to Eq. (4.5). Thus Eq. (4.5) has been justified.

The terms in Eq. (4.4) can be represented by graphs as shown in Fig. 8 through third order. In order to write down the diagram for the corresponding terms in Eq. (4.4), it is only necessary to use the fact that J_n means to add a single line to the $n - 1$ lines present, antisymmetrize the incoming and outgoing lines, and multiply by n. The process of antisymmetrization means to connect the lines up in all possible ways with a minus (plus) sign for an odd (even) permutation, and then divide by $n!$. The operation F_n is applied to $n + 1$ lines and means to connect the top outgoing line with the second incoming line, after crossing the first incoming line. Then the n incoming lines are antisymmetrized. Since, from Eq. (4.5), the terms of arbitrary order can be obtained in terms of the F's and J's, the above rules for constructing the diagrams can be used in a systematic manner. In Fig. 8 the graphs for the corresponding terms in Eq. (4.4) are shown to third order.

Fig. 8 can be simplified considerably by noting that the lines coming out from a vertex are equivalent. If they are exchanged, a minus sign is needed, because the matrix element at the vertex is antisymmetric. The same is true for the two incoming lines. The situation is illustrated in Fig. 9.

The diagrams in Fig. 8 can be simplified further by eliminating the repeated antisymmetrizations. If a group of $n - 1$ lines is antisymmetrized, and another line is added and all n are antisymmetrized, the first antisymmetrization is not needed. This situation is shown graphically in Fig. 10 for four lines.

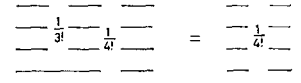
Therefore, using the rules illustrated in Figs. 9 and 10, Fig. 8 can be simplified as shown in Fig. 11. The problem now is to connect the lines in all possible ways with a minus (plus) sign for an odd (even) permutation. The connection can be made graphically for the first- and second-order graphs, but becomes more cumbersome in the case of third order. The problem of connection can be simplified by using the permutation group and the fact that two lines coming out from a vertex are equivalent.

For the first-order diagram, the only group of permutations which must be considered is the symmetric group $S_2 = \{e, (12)\}$. However, (12) gives the same graph as e if one of the lines going out from the vertex is crossed over the other one. This process gives a factor (-1) which combines with the (-1) due to (12) being an odd permutation. Therefore, it is only necessary to consider e and multiply the graph by a factor 2 as is done in Fig. 12 for first order.

The second-order term can be treated similarly. It is the symmetric group

$$S_3 = \{e, (12), (13), (23), (132), (123)\}$$

FIG. 10. Example of the redundancy of repeated antisymmetrizations.



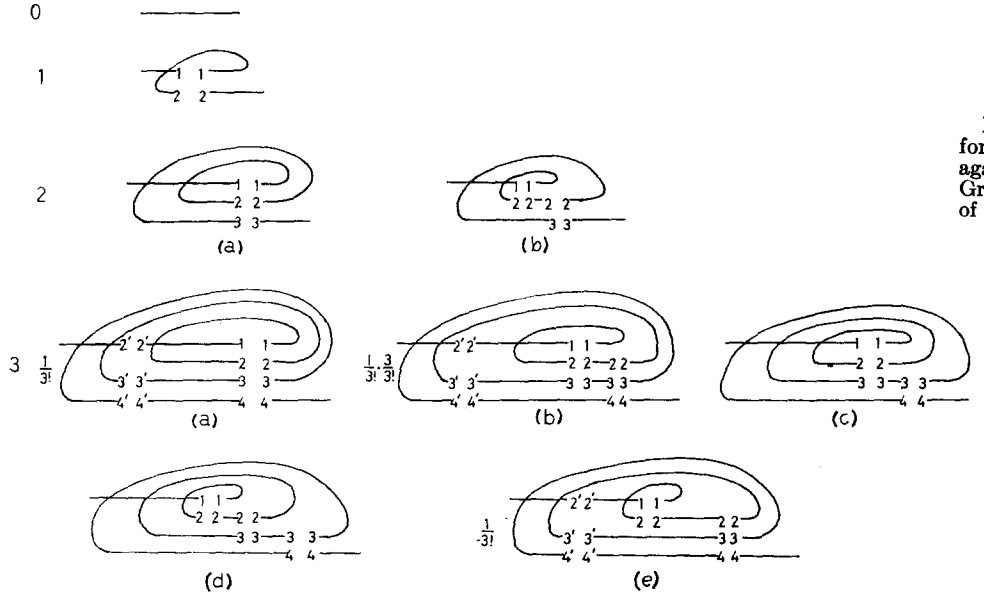


FIG. 11. Reduced diagrams for the single-particle propagator obtained from the Green's functions equations of motion.

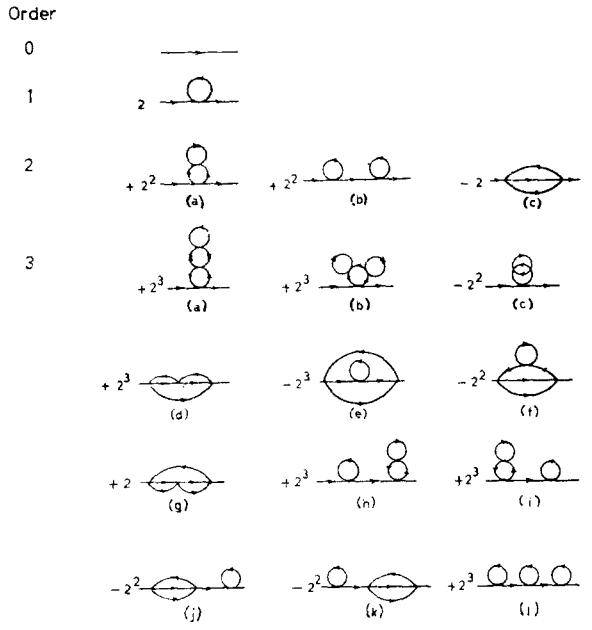


FIG. 12. Topologically different graphs for the single-particle propagator obtained from the diagrams of Fig. 11.

which must be considered. However, it is only the left cosets of the subgroup S_2 which give different diagrams. The left cosets of S_2 are $2a = \{e, (12)\}$, $2b = \{(23), (132)\}$, and $-2c = \{(13), (123)\}$ which correspond to the graphs in Fig. 12 (2), respectively. Since each of the elements in a coset gives the same graph, it is multiplied by two. After making a permutation, the graph is multiplied by the sign of the permutation and then put in the form shown in Fig. 12 by crossing the lines coming out or going in to each vertex, if necessary. There is a factor of (-1) for each crossover, because the matrix element is antisymmetric. Therefore, the graph c in Fig. 12 (2) is multiplied by (-1), since the permutation (13) is odd and two crossovers are necessary.

The graph in Fig. 11 (2a) corresponds to the full symmetric group S_3 and therefore contributes $2a + 2b - 2c$. The graph in Fig. 11 (2b) corresponds to the product

$$\{e, (23)\} \cdot \{e, (12)\} = \{e, (12), (23), (132)\} = 2a + 2b.$$

Thus, the total second-order contribution is $2^2a + 2^2b - 2c$ as shown in Fig. 12 (2).

The third-order term in Fig. 11 is more complicated, because the graphs in Fig. 11 [3(a, b, e)] must also be connected with respect to the primed numbers (2′, 3′, 4′) as well as the unprimed numbers (1, 2, 3, 4). However, the connection can be facilitated by considering the left cosets of the subgroup $\{e, (12)\}$ and the subgroup $\{e', (2'3')\}$. Then each coset corresponds to a graph, and the number of permutations that must be considered is reduced from 144 by a factor of four to 36. When the connections are made in this manner, taking into account the proper sign, the graphs shown in Fig. 12 (3) are obtained.

One of the main advantages of this method over the Wick's theorem method is that there is no danger of leaving out a topologically different graph. In fact, all the topologically different linked graphs are obtained from the diagrams of the type shown in Fig. 11(a), since the other diagrams just represent restrictions on the ways of connecting the lines. The other diagrams are of course essential for determining the factors associated with topologically different graphs, but will not generate any new ones.

The graphs shown in Fig. 12 are Hugenholtz graphs[6], since the interaction is represented by a vertex instead of a dotted line. In order to obtain Goldstone-type[6] graphs, it is only necessary to substitute Fig. 13 into Fig. 12 for the vertices. The first figure on the right side of Fig. 13 is the direct term and the second term is the exchange term. The advantage of Hugenholtz vertices over Goldstone vertices is apparent when one considers that in first order there is just one Hugenholtz graph *versus* two Goldstone graphs, in second order it is 3 *vs* 10, and in third order it is 12 *vs* 74. Klein and Prange,[3] who used Goldstone vertices, give the ten different linked second-order graphs.[22] In Fig. 12 there are no unlinked graphs, which illustrates the linked cluster theorem proved in the last section.

The self-energy function is extremely important when calculating the energy shift in the single-particle (hole) energies.[2] It can also be used in connection with the single-particle propagator to calculate the ground-state energy.[3] The terms in Fig. 12 (1), (2a, c), (3a,-g) are irreducible graphs, and therefore contribute to the self-energy function.

The rules for the mathematical contribution from the graphs in Fig. 12 can be obtained from Eqs. (2.13), (2.14), and (2.15), where the operators F_n and J_n of Eq. (3.1) are defined. In Eq. (4.2), for every F_k there is a J_{k+1}. Since both have a factor $(-1)^k$, this factor does not contribute. The vertex is given by the h factor in Eq. (2.14), and the lines are given by G^0 in Eq. (2.15). In addition, there is a factor $-i$ for each J appearing in the term. The factor

[22] Schultz (Ref. 2, p. 53) gives ten different Goldstone linked graphs with unlinked parts in second order. Abrikosov *et al.* also give ten different Goldstone second-order graphs (Ref. 2, p. 73) and three different Hugenholtz second-order graphs (Ref. 2, p. 76).

obtained from connecting the diagrams of Fig. 11 together is $2^{p-m}(-1)^{p+f}$, where p is the order, m is the number of pairs of equivalent lines, and f is the number of closed loops. This factor can be seen to be valid through third order by looking at Fig. 12. It will be justified to all orders later.

The graph in Fig. 12 (1) is considered to be a closed loop, so it is clear that the graphs in Fig. 12 [2(a, b)] have two closed loops and the graphs in Fig. 12 [3(a, b, h, i, l)] have three closed loops. The graph of Fig. 12 (2c) is considered also to have just one closed loop, since there is only one distinct path leaving one vertex and returning to it. The closed loop can be seen even more clearly, if the direct part of the Goldstone interaction in Fig. 13 is substituted for the Hugenholtz vertices. If there is any doubt about the number of closed loops in a Hugenholtz graph, the direct part of the Goldstone interaction can always be substituted for the vertex and the actual number of closed loops can be easily counted. This method shows that the number of closed loops in Figs. 12 [3(c, e, f, j, k)] is two, and the number of closed loops in Figs. 12 [3(d, g)] is one.

A pair of equivalent lines are two lines that can be interchanged without changing the appearance of the graph. Thus, in Fig. 12 (2c), the two bottom lines form a pair of equivalent lines. Likewise, the graphs in Figs. 12 [3(c, f, j, k)] have a pair of equivalent lines, and the graph of Fig. 12 (3g) has two pairs. All the others have no equivalent lines.

The rules for obtaining the one-particle Green's function can thus be stated in the following way:

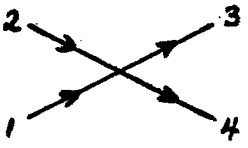
(1) Draw all topologically different linked graphs having one line in and one line out with arrows.

(2) For each line $\overrightarrow{1\quad 2}$ associate a factor

$$\delta_{12}[\omega_1 - e_1 + i0_1]^{-1},$$

where

$$0_1 = \begin{cases} +0, & \text{if} \quad k_1 > k_F, \\ -0, & \text{if} \quad k_1 < k_F. \end{cases}$$

(3) For each vertex 

associate a factor

$$\langle 12|\ V\ |34\rangle \times \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4) \exp(-i\omega_3\epsilon + i\omega_2 2\epsilon).$$

(4) Integrate (sum) over the internal frequencies (momenta, spin).

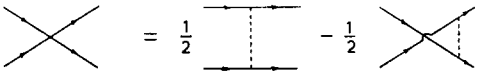


FIG. 13. The connection between the Hugenholtz interaction vertex and the Goldstone interaction.

(5) Multiply by an overall factor

$$[(-2\pi)^{2p+1}][(2\pi)^{-3p}2^{-p}][2^{p-m}(-1)^{p+f}][(-i)^{p+1}]i = (-2\pi)(i/2\pi)^p(-1)^f 2^{-m},$$

where f is the number of closed loops and m is the number of pairs of equivalent lines.

The overall factor in rule (5) is composed of various parts. The first square bracket with $(-2\pi)^{2p+1}$ is due to the $(2p + 1)$ G^0's since there are p F's and $(p + 1)$ J's. The next square bracket comes from the vertex function in Eq. (2.14), which gives the factor $[(2\pi)^{-3}2^{-1}]p$ times. The third square bracket comes from the ways of connecting the diagrams of Fig. 11 and will be justified below. The $(-i)^{p+1}$ comes from the $(p + 1)$ J's and the i is from the L_0.

These rules are essentially the same as the ones stated by Nozières and by Abrikosov, *et al.*[23] It is not necessary to add another rule to take graphs with closed loops of the type shown in Fig. 12 (1) into account, since the exponential factors in rule (3) are equivalent to saying that the integration must be in the upper half plane. This exponential factor is due to the ordering of the operators in the Heisenberg equation of motion (see the Appendix).

From the equation of motion method, all these rules have been deduced to all orders except for the factor $2^{p-m}(-1)^{p+f}$ in rule (5). This factor has been shown to be valid through third order, and will now be shown to be valid to arbitrary order.

The sign factor $(-1)^{p+f}$ will now be established by induction. By examining the $(p + 1)$st-order diagrams of the type shown in Fig. 11(a), it can be seen that the graphs with a closed loop of the type shown in Fig. 12 (1) will have the same sign as the corresponding pth-order graph without the loop. If $1 \to 1$, we get a closed loop without a sign change. If $k \to k - 1$ for $k = 2, 3, \cdots, p + 1$ and $k' \to k'$, $k'' \to k''$, $\cdots$ then a closed loop will be formed if one of the lines going out from the vertex is crossed over the other, as shown in Fig. 14(a). This crossover gives a factor (-1) which combines with the (-1) obtained from the transposition $k \to k - 1$ to give unity. Other ways of obtaining the closed loops of Fig. 12 (1) are equivalent to this way. Thus, in $(p + 1)$st-order, the sign factor is

[23] The rules are given by Nozières in Ref. 2, p. 185, and by Abrikosov *et al.* (Ref. 2, p. 76). See also Ref. 3.

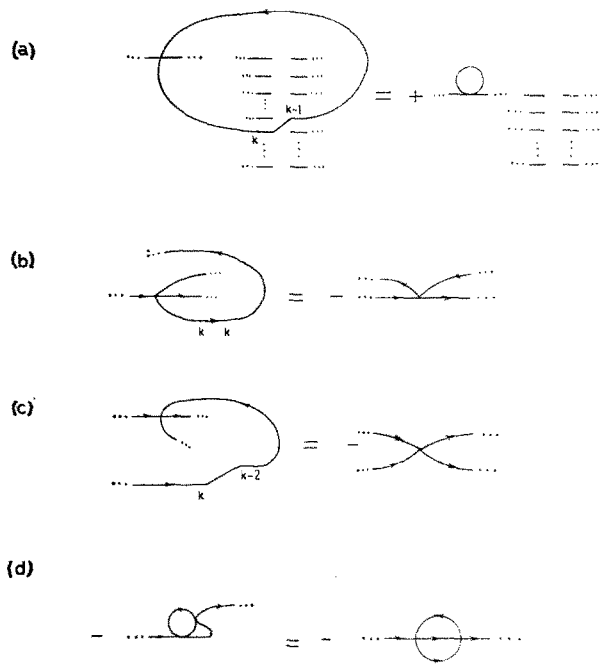


FIG. 14. Diagrams used for establishing the rule for the $(-1)^{p+f}$ sign factor.

$(-1)^{p+f} = (-1)^{(p+1)+(f+1)}$ which is correct because there is one more closed loop.

Before the closed loop of the type shown in Fig. 12 (2c) is considered, the types of scattering that can be obtained will be first considered. The diagram shown in Fig. 14(b) can be regarded as a subdiagram of a larger diagram, and it can be rearranged as a scattering between particle and hole as shown on the right side. There is a minus sign because one crossover is necessary and the original permutation is $k \to k$, $k' \to k'$, $\cdots$. The diagram of Fig. 14(c) can also occur as part of a larger diagram and can be rearranged to give scattering between two particles with a minus sign, because one crossover is necessary and the original permutation is $k \to (k-2)$, $k' \to k'$, $\cdots$. Thus, when these scatterings are added to a pth-order graph, no new closed loops are considered to be formed and the sign of the new graph is $(-1)(-1)^{p+f} = (-1)^{(p+1)+f}$. The graph of Fig. 12 (3d) is interpreted as having only one closed loop, as can be seen by drawing the corresponding Goldstone graph.

The closed loop of the type shown in Fig. 12 (2c) can be obtained by combining a scattering of the type shown in Fig. 14(c) with the closed loop of Fig. 12 (1) as shown in Fig. 14(d). The sign of the new graph will be $(-1)(-1)^{p+f} = (-1)^{(p+1)+f}$, since one closed loop will be destroyed and another one created. Thus, the number of closed loops will be the same and the correct sign will be obtained. Therefore, the sign $(-1)^{p+f}$ has been established by induction.

The factor 2^{p+m} used in obtaining rule (5) can also be established by induction. It is true for zeroth, first, second, and third orders, and will be assumed true for the pth-order. If we have the pth-order terms in Eq. (4.5), then the $(p+1)$st-order terms can be obtained by making the replacement

$$\begin{aligned} J_k \cdots J_1 \to\ & F_k J_{k+1} J_k \cdots J_1 \\ & + J_k F_{k-1} J_k J_{k-1} \cdots J_1 + \cdots \\ & + J_k \cdots J_{k-p} F_{k-p-1} J_{k-p} \cdots J_1 \\ & + \cdots + J_k \cdots J_2 F_1 J_2 J_1 \end{aligned} \tag{4.10}$$

in the last uninterrupted series of J's in each term. This procedure can be seen to be valid for zeroth, first, second, and third order from Eq. (4.4). If an arbitrary $(p+1)$st-order term is considered, and the first FJ term encountered in going from the right to the left is removed, the result would be one of the pth-order terms. Thus, all the $(p+1)$st-

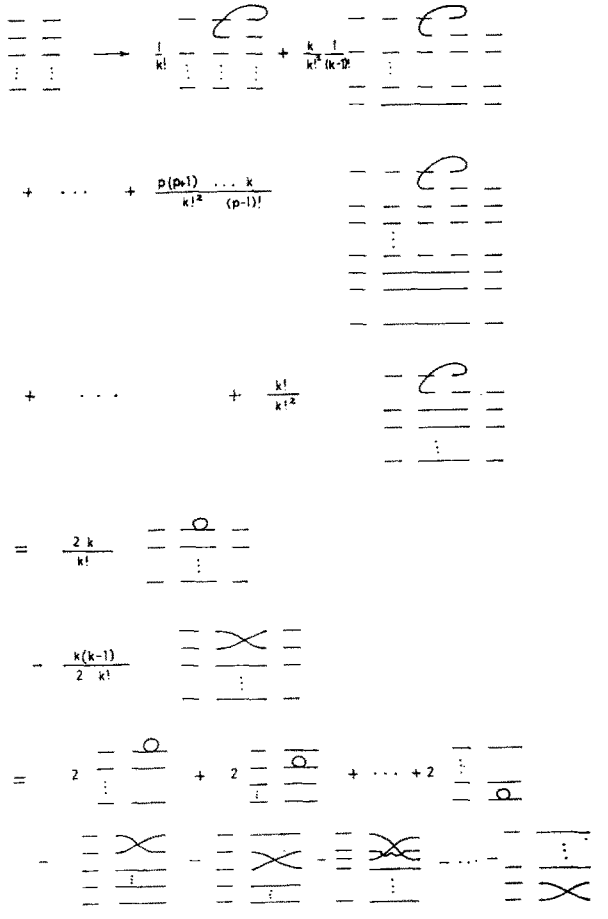


FIG. 15. Insertion made to obtain the next higher-order diagrams.

order terms are generated in this way. Equation (4.10) is shown diagrammatically in Fig. 15. If the lines are connected as indicated, the result shown in the last line is obtained. It says that, in the diagrams of Fig. 11, the lines after the last interaction on the right are replaced with loops of the type of Fig. 12 (1) in all possible ways with a factor 2, and are also allowed to scatter with each other in all possible ways. The way in which these insertions are made in the pth-order diagrams of the type of Fig. 11 guarantees that the graphs in $(p+1)$st-order will have the correct factors. If a loop of the type in Fig. 12 (1) is inserted into a pth-order graph with a factor 2^{p-m} the resulting graph will have a factor $2^{(p+1)-m}$ as shown in Fig. 16(a). If the two lines coming out from a vertex in a pth-order graph are allowed to scatter, the resulting graph will have the factor $2^{p-m} = 2^{(p+1)-(m+1)}$, because one more pair of equivalent lines has been formed as shown in Fig. 16(b). If a pair of equivalent lines is destroyed by the insertion of a loop in each of the lines as shown in Fig. 16(c), the resulting factor will be $2\cdot 2\cdot 2^{p-m} = 2^{(p+1)-(m-1)}$ because the resulting graph will have one less pair of equivalent lines. It is also possible for a pair of equivalent lines to be destroyed in the way shown in Fig. 16(d). The same $(p+1)$st-order graph can be obtained by allowing the top line to scatter with the middle line or the bottom line in the first graph on the left side. It can also be obtained by allowing the two closed loops in the second graph on the left side to scatter with each other. When these contributions are combined, the result is the $(p+1)$st-order graph with the proper factor $2^{(p+1)-m}$.

In order to complete the induction proof, it is necessary to show that the restrictions in the ways of connecting the lines of the diagrams in Fig. 11 will guarantee that no $(p+1)$st-order graph will be produced twice, by different insertions in different pth-order graphs. This hypothesis has been verified up to third order, but the general proof has not been carried out. The previous discussion has, however, given some insight into the problem and made the factor 2^{p-m} in rule (5) reasonable. Since this factor is obtained by the Wick's theorem method,[2] the hypothesis must be true.

The equation of motion method is an alternative way of obtaining the single particle Green's function. Nozières[2] states that the principal difficulties in the Wick's theorem approach are not to leave out graphs and to calculate the factor properly. Abrikosov *et al.* state that, for higher-order terms, it is best not to rely on the rules for drawing the

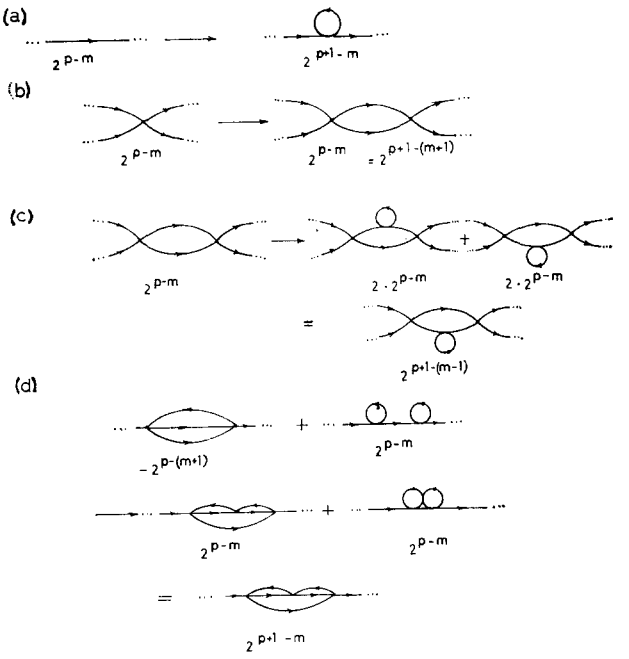


FIG. 16. Diagrams used in establishing the rule for the 2^{p-m} factor.

graphs but to return to the expression for the Green's function in the interaction picture, and use Wick's theorem directly with the graphs only as guides.[24] The method based on the equations of motion has the advantage over the Wick's theorem method in that explicit diagrams of the type shown in Fig. 11 can be drawn to generate all topologically different linked graphs with the proper factors. The unlinked graphs are avoided, which is an advantage since they are not physical. In the next section, it will be shown that the method is also applicable to the two-particle Green's function.

V. THE TWO-PARTICLE GREEN'S FUNCTION

The two-particle Green's function is very important in determining collective excitations,[2] so it is of interest to see if it can be calculated from the method presented here. Eq. (3.21) for G_2 gives the expansion

$$\begin{aligned} G_2 = {} & K_2J_2J_1i \\ & + K_2F_2K_3J_3K_2J_2J_1i \\ & + K_2F_2K_3F_3K_4J_4K_3J_3K_2J_2J_1i \\ & + K_2F_2K_3F_3K_4F_4K_5J_5K_4J_4K_3J_3K_2J_2J_1i \\ & + K_2F_2K_3F_3K_4F_4K_5F_5K_6J_6 \\ & \times K_5J_5K_4J_4K_3J_3K_2J_2J_1i + \cdots . \end{aligned} \tag{5.1}$$

[24] See Abrikosov *et al.* (Ref. 2, p. 76, footnote 12).

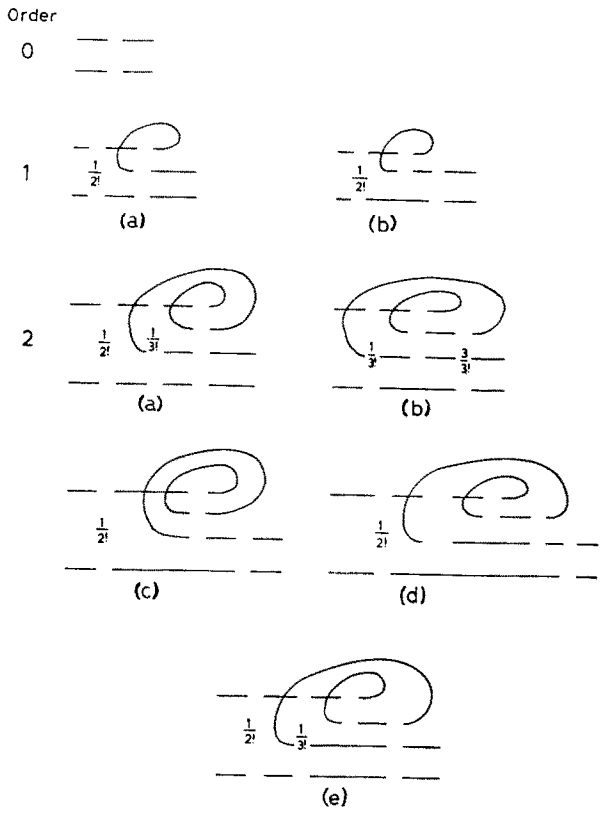


FIG. 17. The diagrams for the two-particle Green's function obtained from the equations of motion.

When the expansions for K_2, K_3, K_4, $\cdots$ in Eq. (4.3) are substituted into Eq. (5.1), and when the terms are collected according to order, the result is

$$\begin{aligned} G_2 = {} & J_2J_1i + \{J_2F_1 + F_2J_3\}J_2J_1i \\ & + \{J_2F_1J_2F_1 + J_2F_1F_2J_3 + F_2J_3F_2J_3 \\ & + F_2J_3J_2F_1 + F_2F_3J_4J_3\}J_2J_1i \\ & + \cdots . \end{aligned} \tag{5.2}$$

Eq. (5.2) can be written in a more complete and concise form as

$$G_2 = \sum_{n=0}^{\infty} [\text{distinct permutations of } nF\text{'s and } nJ\text{'s}]J_2J_1i \tag{5.3}$$

if the terms in the expansion are subscripted according to the number of lines remaining after the application of the operator, and if the operators with nonpositive subscripts are set equal to zero. The number of lines coming in and going out must be two, of course.

The expansion in Eq. (5.3) can be proved by considering an arbitrary pth-order term and looking at the maximum value of the subscript on F, say k. This term therefore must have the basic structure $F_2F_3 \cdots F_kJ_{k+1}J_k \cdots J_1i$ without considering the K's in Eq. (5.1). Because of the K's in Eq. (5.1), an insertion of the type shown in Eq. (4.9) is allowed between any or all of the operators as long as the total number of F's is p and as long as all subscripts are positive. Thus, an arbitrary term in Eq. (5.3) corresponds to a definite term in the expanded form of Eq. (5.1). Likewise, an arbitrary term in the expanded form of Eq. (5.1) corresponds to a definite term in Eq. (5.3).

The terms in Eq. (5.2) are shown in Fig. 17. The diagrams can easily be drawn by remembering the definitions of the operators F and J in Eq. (3.1). The diagrams to an arbitrary order can be constructed with the help of Eq. (5.3).

When the diagrams of Fig. 17 are connected in all possible ways, the resulting graphs obtained are shown in Fig. 18. In connecting the diagrams in Fig. 17, it is convenient to group the allowable permutations into cosets of the subgroup $\{e, (12), (34), (12)(34)\}$, because the lines going out are equivalent if they are antisymmetrized.

The rules for obtaining the mathematical contribution of the topologically different graphs in Fig. 18 are the same as for G_1, except that rule (1)

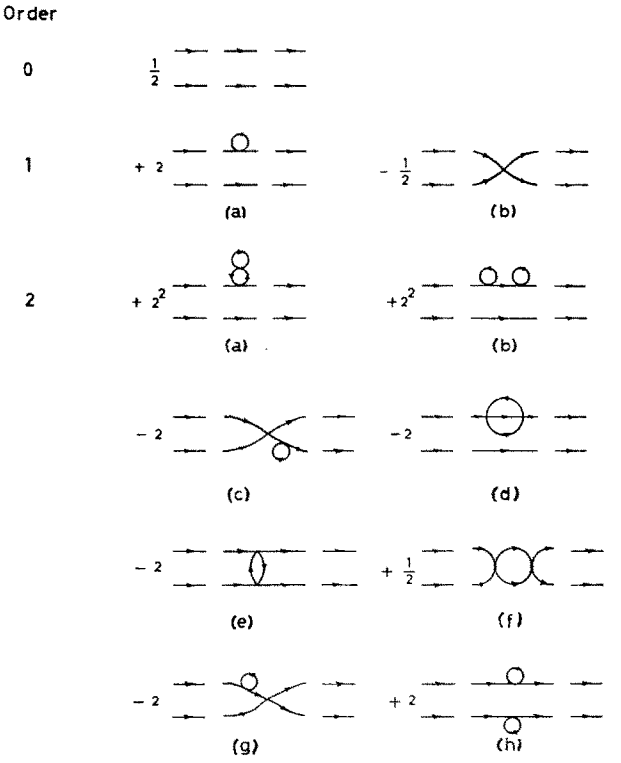


FIG. 18. The topologically different graphs for the two-particle Green's function through second order.

must be changed to drawing all topologically different graphs with two lines in and two lines out as shown in Fig. 18. There is an additional factor of $(-2\pi)(-i)$ in rule (5) because there is one more J in the expression. The rules are thus essentially the same as stated by Nozières.[25]

VI. CONCLUSION

In this paper an alternative to the usual many-particle perturbation theory for the Green's function[2] based on Wick's theorem is developed. The treatment here goes beyond that of Klein and Prange[3] in that the linked cluster theorem is shown to be valid for any Green's function. In other words, unlinked graphs do not contribute to any Green's function. The formalism was illustrated by calculating the one-particle Green's function to third order, and the two-particle Green's function to second order. The advantage of the diagrams used here is that all the topologically different graphs can be generated with the correct factors. Thus, there is no danger of leaving out a topologically different graph or getting the wrong factor associated with a graph. In higher-order terms, the program becomes somewhat tedious, but it is straightforward. Group theory can be used to simplify the connections somewhat by classifying the graphs according to equivalent cosets of the permutation groups. The presentation here avoids the unphysical unlinked terms and is somewhat simpler than the usual perturbation treatment with which this presentation is in agreement.

ACKNOWLEDGMENTS

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APPENDIX. DERIVATION OF THE EQUATION OF MOTION

Because the equation of motion for the Green's functions are so important, they will be derived here in more detail. The operator Z_1 in Eq. (2.8) involved a differentiation with respect to time, so we can differentiate Eq. (2.4) with respect to t_1.

$$
\begin{aligned}
&i\frac{\partial}{\partial t_1}\mathcal{G}_n(1, 2, \cdots, 2n) \\
&= i\langle N|\, T\left\{i\frac{da_1}{dt_1}\, a_2 \cdots a_n a_{n+1}^{+} \cdots a_{2n}^{+}\right\}|N\rangle \\
&\quad - \langle N|\frac{\partial T}{\partial t_1}\{a_1 \cdots a_n a_{n+1}^{+} \cdots a_{2n}^{+}\}|N\rangle. \qquad \text{(A1)}
\end{aligned}
$$

The last term represents symbolically the differentiation of the time-ordering operator. The equation of motion for the annihilation operator in the Heisenberg picture, obtained from Eqs. (2.5) and (2.1), is

$$
\begin{aligned}
&i\, da_1/dt_1 = [a_1, H] \\
&\quad = e_1 a_1 + \tfrac{1}{2}\sum{}'\langle 12'|\, V\,|3'4'\rangle a_2^{+} a_{3'} a_{4'}. \qquad \text{(A2)}
\end{aligned}
$$

If Eq. (A2) is substituted into Eq. (A1), the result can be written as

$$
\begin{aligned}
&\left(i\frac{\partial}{\partial t_1} - e_1\right)\mathcal{G}_n \\
&= \sum{}'\int_{-\infty}^{\infty}\!\!\int\!\!\int dt_2'\, dt_3'\, dt_4'\, \tfrac{1}{2}\langle 12'|\, V\,|3'4'\rangle(-1)^{n+1} \\
&\quad \times \delta(t_2' - t_1 - 2\epsilon)\,\delta(t_3' - t_1 - \epsilon)\,\delta(t_4' - t_1) \\
&\quad \times \mathcal{G}_n(3'4'2 \cdots n; 2', n+1, \cdots 2n) \\
&\quad - \langle N|\, \partial T/\partial t_1\,|N\rangle. \qquad \text{(A3)}
\end{aligned}
$$

The differentiation of the time-ordering operator has not been explicitly given in the literature, so it will be given here. It can be obtained by differentiating the step functions in Eq. (2.6)

$$
\begin{aligned}
&i\langle \partial T/\partial t_1\rangle \\
&= i\sum_{P'}(-1)^{P'}P'\langle A_1 A_2 \cdots A_{2n}\rangle \\
&\quad \times \delta(1-2)\theta(2-3)\cdots\theta((2n-1)-2n) \\
&\quad + i\sum_{P'}(-1)^{P'}P'\langle A_2 A_1 A_3 \cdots A_{2n}\rangle \\
&\quad \times \delta(2-1)\theta(1-3)\cdots\theta((2n-1)-2n) \\
&\quad - i\sum_{P'}(-1)^{P'}P'\langle A_2 A_1 A_3 \cdots A_{2n}\rangle \\
&\quad \times \theta(2-1)\,\delta(1-3)\theta(3-4)\cdots\theta((2n-1)-2n) \\
&\quad - i\sum_{P'}(-1)^{P'}P'\langle A_2 A_3 A_1 \cdots A_{2n}\rangle \\
&\quad \times \theta(2-3)\,\delta(3-1)\theta(1-4)\cdots \\
&\quad + i\sum_{P'}(-1)^{P'}P'\langle A_2 A_3 A_1 A_4 \cdots A_{2n}\rangle \\
&\quad \times \theta(2-3)\theta(3-1)\,\delta(1-4)\theta(4-5)\cdots \\
&\quad + \cdots \qquad \text{(A4)}
\end{aligned}
$$

[25] See Nozières (Ref. 2, p. 185).

or

$$i\langle\partial T/\partial t_1\rangle = i\sum_{P'}(-1)^{P'}P'\ \delta(1-2)\langle(A_1A_2+A_2A_1)A_3\cdots A_{2n}\rangle\theta(2-3)\theta(3-4)\cdots$$
$$-i\sum_{P'}(-1)^{P'}P'\ \delta(1-3)\langle A_2(A_1A_3+A_3A_1)A_4\cdots A_{2n}\rangle\theta(2-3)\cdots$$
$$+\cdots, \tag{A5}$$

where P' is a permutation of the numbers $2, 3, \cdots, 2n$. If the anticommutation relations of Eq. (2.3) are used the result is

$$i\langle\partial T/\partial t_1\rangle = i\sum_{P'}(-1)^{P'}P'\ \delta_{12}\ \theta(2-n)\langle A_2\cdots A_{2n}\rangle$$
$$\times[\theta(2-3)\theta(3-4)\cdots$$
$$+\theta(3-2)\theta(2-4)\cdots$$
$$+\theta(3-4)\theta(4-2)\cdots$$
$$+\cdots]. \tag{A6}$$

By considering all possible values of t_2, the step functions in the square bracket in Eq. (A6) can be written as just

$$\theta(3-4)\theta(4-5)\cdots\theta((2n-1)-2n).$$

Eq. (A6) can then be written in the more convenient form

$$i\langle\partial T/\partial t_1\rangle = \sum_{k=n+1}^{2n}(-1)^k\ \delta_{1k}$$
$$\times\mathcal{G}_{n-1}(2,\cdots k-1, k+1,\cdots,2n). \tag{A7}$$

If Eq. (A7) is substituted into Eq. (A3) and the result is substituted into $Z_1\mathcal{G}_n$, we obtain

$$\mathcal{G}_n(1,2,\cdots,2n) = -ie^{-ie_1t_1}\int_{-\infty}^{\infty}dt_1'\,[(1-c_1)\theta(t_1-t_1')-c_1\theta(t_1'-t_1)]e^{ie_1t_1'}$$
$$\times\Big\{\sum{}'\tfrac{1}{2}\langle 12'|\ V\ |3'4'\rangle(-1)^{n+1}\ \delta(t_2'-t_1'-2\epsilon)\ \delta(t_3'-t_1'-\epsilon)$$
$$\times\delta(t_4'-t_1')\mathcal{G}_{n+1}(3'4'2\cdots n;2',n+1,\cdots 2n)$$
$$+\sum_{k=n+1}^{2n}i\ \delta_{1'k}(-1)^k\mathcal{G}_{n-1}(2,\cdots,k-1,k+1,\cdots,2n)\Big\}. \tag{A8}$$

If the Fourier transform operator of Eq. (2.11) is now applied to Eq. (A8) and use is made of the representation of the delta function

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}dy\,e^{ixy} \tag{A9}$$

and the step function

$$\theta(x) = \frac{i}{2\pi}\int_{-\infty}^{\infty}dy\,e^{-ixy}(y+i0)^{-1}, \tag{A10}$$

the result is

$$G_n = \sum{}'(-1)^n h(1'2'3'4')G^0(1,1')G_{n+1}(3'4'2\cdots n,2',n+1,\cdots 2n)$$
$$-i\sum_{k=n+1}^{2n}(-1)^kG^0(1,k)G_{n-1}(2,\cdots k-1,k+1,\cdots 2n). \tag{A11}$$

In Eq. (A11) the quantity h is defined by Eq. (2.14), and the single-particle propagator is defined by Eq. (2.15). By antisymmetrizing and writing the sum in terms of the antisymmetrization operator, Eq. (2.13) is obtained for the Green's function equation of motion.

A Remark on a Reducible Quantum Field Theory with a One-Parameter Symmetry Group

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The connection between certain symmetry properties of a reducible algebra generated by the field operator and the decomposition into irreducible algebras is exhibited.

1. INTRODUCTION

WE investigate a reducible, scalar, charged quantum field in a separable Hilbert space together with a one-parameter compact symmetry group. The situation is similar to that considered in a previous paper,[1] but the restrictions imposed on the field are relaxed as compared to Sec. 3 of Ref. 1.

The statement proven below establishes the connection between the properties of the field and the symmetry group on one hand, and the reduction of the algebra with respect to the commutant on the other hand. Roughly speaking, the one-parameter compact symmetry group gives the connection between the reduced spaces and algebras generated by the field, provided that the original algebra, together with the symmetry group, is irreducible.

This is a step forward compared with the result of Sec. 3 of Ref. 1. In Ref. 1 we proved only the reverse statement which reads as follows: Suppose the symmetry group is such that it maps the reducing spaces isometrically and the reduced algebras in an inequivalent way into each other, then the reducible algebra together with the symmetry group form an irreducible algebra. This statement, as presented in Ref. 1, was proved by using the usually stated axioms for the field. Notice that in this paper we do not need to appeal to all axioms of field theory. This makes it possible to apply the result of Secs. 2 and 3 to nonrelativistic, and nonlocal, theories.

2. ASSUMPTIONS AND THEOREM

We assume the following: Let $\mathfrak{R}$ denote a cyclic reducible uniformly closed symmetric algebra of bounded operators in a separable Hilbert space $\mathfrak{H}$ corresponding to a reducible quantum field theory. $\phi_0 \in \mathfrak{H}$ denotes a cyclic vector. The commutant $\mathfrak{R}'$ of $\mathfrak{R}$ is assumed to be Abelian. $\{G(\beta)\} = \mathfrak{G}$ denotes the unitary representation of a one-parameter compact group, $G(\beta + 2\pi) = G(\beta)$, $G(0) = I$, $G(\beta)$ weakly continuous in B.[2]

The cyclic vector ϕ_0 is assumed to be an eigenstate of $G(\beta)$ for all β. Finally, $\mathfrak{R}$ and $\mathfrak{G}$ are assumed to fulfill

$$G(\beta)\mathfrak{R}G^+(\beta) \subset \mathfrak{R},$$

i.e., $\mathfrak{G}$ maps $\mathfrak{R}$ into $\mathfrak{R}$, and if $\{\mathfrak{R}, \mathfrak{G}\}$ denotes the algebra generated by the union of $\mathfrak{R}$ and $\mathfrak{G}$,

$$\{\mathfrak{R}, \mathfrak{G}\}' = \lambda I,$$

i.e., irreducibility of the union.

Statement: Under the above-mentioned assumptions there exists a decomposition of $\mathfrak{H}$ into a direct integral

$$\mathfrak{H} = \int_0^{2\pi\oplus} \mathfrak{H}_\alpha (d\alpha)^{\frac{1}{2}},$$

$$\mathfrak{R} = \int_0^{2\pi\oplus} \mathfrak{R}_\alpha,$$

$$\mathfrak{R}' = \left\{ \int_0^{2\pi\oplus} f(\alpha) \cdot I_\alpha \right\},$$

such that

$$G(\beta) \int_\Delta^\oplus I_\alpha G^+(\beta) = \int_\Delta^\oplus I_{\alpha+n\cdot\beta}. \tag{1}$$

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[1] J. Lopuszanski and H. Reeh, J. Math. Phys. 7, 148 (1966).

[2] The representation of the one-parameter compact group is unitary. According to Stone's theorem [see, for example, F. Riesz and B. Sz. -Nagy, *Functional Analysis* (Frederick Ungar Publishing Company, New York, 1955)], $G(\beta) = \exp iQ\beta$, where Q is a self-adjoint operator. Because of the periodicity condition $G(\beta) = G(B + 2\pi)$, the spectrum of Q is discrete and consists of integers. This spectrum cannot be bounded either from below or from above, unless $G(\beta)$ commutes element-wise with the Abelian commutant $\mathfrak{R}'$; this follows in an anlogous way as a theorem proved by Araki for the translational group. See H. Araki, Progr. Theoret. Phys. (Kyoto) 32, 844 (1964); see also M. Guenin, J. Math. Phys. 7, 271 (1966).

[I_α denotes the identity operator on $\mathfrak{H}_\alpha$, $f(\alpha)$ is a Lebesgue-measureable essentially bounded function, Δ any subinterval of the interval $(0, 2\pi)$, the dependence of α is always modulo 2π; $n = \pm 1, \pm 2, \cdots$.]

3. PROOF OF THE THEOREM

(A). $\mathfrak{G}$ does not commute with any element in $\mathfrak{R}'$ except multiples of the unity, since otherwise $\{\mathfrak{R}, \mathfrak{G}\}'$, containing all elements in $\mathfrak{R}'$ commuting with $\mathfrak{G}$, would not be a multiple of unity.

(B). We have

$$G(\beta)\mathfrak{R}'G^+(\beta) \subset \mathfrak{R}';$$

namely, if $B \in \mathfrak{R}'$ and $A \in \mathfrak{R}$, then

$$G(\beta)BG^+(\beta)A - AG(\beta)BG^+(\beta) = C,$$

$$G^+(\beta)CG(\beta) = BG^+(\beta)AG(\beta) - G^+(\beta)AG(\beta)B = B\hat{A} - \hat{A}B = 0,$$

since $\hat{A} \in \mathfrak{R}$; therefore $C = 0$.

(C). We can decompose $\mathfrak{H}$ with respect to the Abelian $\mathfrak{R}'$ in the following way[3]

$$\mathfrak{H} = \int^{\oplus} \mathfrak{H}_\alpha (d\rho(\alpha))^{\frac{1}{2}}, \qquad \mathfrak{R} = \int^{\oplus} \mathfrak{R}_\alpha,$$
$$\mathfrak{R}' = \left\{ \int^{\oplus} f(\alpha) I_\alpha \right\}, \qquad \phi_0 = \int^{\oplus} \phi_{0\alpha}, \ ||\phi_{0\alpha}||^2 = 1. \tag{2}$$

Here α is running over a finite segment of the real axis containing the spectrum of an operator A generating $\mathfrak{R}'$, $\rho(\alpha) = (\phi_0 \mid E_\alpha \phi_0)$ is given by the spectral resolution of that operator (we may assume $\int d\rho\ (\alpha) = 1$), $f(\alpha)$ denotes an essentially bounded $\rho(\alpha)$ measurable function, and I_α stands for the identity operator in the Hilbert space $\mathfrak{H}_\alpha$. The reduced algebras $\mathfrak{R}_\alpha$ of the reduced operators in $\mathfrak{H}_\alpha$ are irreducible for almost all α.

(D). By the equivalence of $\mathfrak{R}'$ and the set of functions $\{f(\alpha)\}$, $G(\beta)$ defines a linear one-to-one map of the set $\{f(\alpha)\}$ into itself. We see from (A) that the only $f(\alpha)$ invariant under $\mathfrak{G}$ are $f(\alpha) = \text{const}$ (almost everywhere).

Furthermore, we see that the mappings $f(\alpha) \to f^\beta(\alpha)$ defined by $G(\beta)$ have the property

$$f_1(\alpha)f_2(\alpha) \to f_1^\beta(\alpha)f_2^\beta(\alpha)$$

and are measure-preserving. The first property is an immediate consequence of the fact that the product of two essentially bounded measurable functions is again essential bounded and measurable together with the definition of the mapping. To demonstrate the second assertion, we denote by $f_\Delta(\alpha)$ the characteristic function of a Borel set Δ on the support of ρ. Then by $G(\beta)$

$$f_\Delta(\alpha) \to f_\Delta^\beta(\alpha).$$

If $\{\Delta_i\}$ is a set of pairwise nonintersecting Borel sets covering the whole support of ρ, i.e., $\sum_i f_{\Delta_i}(\alpha) = 1$, then clearly

$$\sum_i f_{\Delta_i}^\beta(\alpha) = 1.$$

On the other hand, we have for $\Delta_i \cap \Delta_k = 0$,

$$f_{\Delta_i}(\alpha)f_{\Delta_k}(\alpha) = 0 = f_{\Delta_i}^\beta(\alpha)f_{\Delta_k}^\beta(\alpha),$$

i.e., supp $f_{\Delta_i}^\beta(\alpha) \cap$ supp $f_{\Delta_k}^\beta(\alpha) = 0$ (up to points of ρ-measure zero). We therefore arrive at

$$f_\Delta^\beta(\alpha) = \begin{cases} 0, \\ 1, \end{cases}$$

which is to say that $f_\Delta^\beta(\alpha) \equiv f_{\Delta_\beta}(\alpha)$ again is a characteristic function of a set Δ_β. If we now look at the vector

$$\int^{\oplus} f_\Delta^\beta(\alpha)\phi_{0\alpha},$$

then the unitarity of $G(\beta)$ and the invarance of ϕ_0 together with $||\phi_{0\alpha}|| = 1$ result in

$$\int_\Delta d\rho\ (\alpha) = \int_{\Delta_\beta} d\rho\ (\alpha).$$

In other words: $G(\beta)$ induces a mapping $\alpha \to \alpha_\beta$ of the points α which is one to one (up to points of ρ-measure zero), ρ measure preserving, and there is no invariant proper subset of points with nonvanishing ρ measure. By $f^\beta(\alpha) = f(\alpha_\beta)$ we have an extension of the mapping induced by $G(\beta)$ to all functions $\in L^1(\rho(\alpha))$,[4] and for f, g, and $f \cdot g \in L^1(\rho(\alpha))$ we have again

$$f(\alpha)g(\alpha) \to f_1^\beta(\alpha)f_2^\beta(\alpha). \tag{3}$$

We denote in the following by $\hat{G}(\beta)$ the unitary representation induced by $G(\beta)$ in $L^2(\rho(\alpha)) \subset L^1(\rho(\alpha))$.

(E). The results of the foregoing paragraph say that the mapping is ergodic; such mappings are well investigated.[5] In particular, we have the following properties: The only invariant functions in $L^1(\rho(\alpha))$ clearly are $f(\alpha) = \text{const}$. Let us look at the eigenfunctions of $\hat{G}(\beta)$ in $L^2(\rho(\alpha))$. Since $\hat{G}(\beta)$ is compact, they form a complete basis and there exists at least one eigenfunction $\varphi_{me}(\alpha)$

$$\hat{G}(\beta)\varphi_{m,e}(\alpha) \equiv \varphi_{m,e}(\alpha_\beta) = e^{im\beta} \cdot \varphi_{m,e}(\alpha)$$

[3] M. A. Naimark, *Normed Rings* (Stechert-Hafner Service Agency, Inc., New York, 1964), Chap. VIII.

[4] E. Hopf, *Ergodentheorie* (Springer-Verlag, Berlin, 1937, and Chelsea Publishing Company, New York, 1948), pp. 4 and 8.

[5] J. von Neumann, Ann. Math. **33**, 587 (1932), and *Collected Works II*, A. H. Taub, Ed. (Pergamon Press, Inc., New York, 1961), p. 307, and Ref. 4.

($||\varphi_{m,e}|| = 1$; for $m \neq 0$, e accounts for a possible degeneracy of the eigenvalue). From this we see that the complex conjugate function $\varphi^*_{m,e}(\alpha)$ belongs to $e^{-im\beta}$, hence it follows by Eq. (3) that $\varphi^*_{m,e}(\alpha)\varphi_{m,e}(\alpha)$ is invariant and therefore equal to a constant, say λ. In particular,

$$\varphi_{m,e}(\alpha)\varphi^*_{m,e}(\alpha) = 1,$$

thus $\varphi_{me}(\alpha) = \lambda\varphi_{me}(\alpha)$, i.e., every eigenvalue is simple.

Denote by n the smallest $m > 0$. By (3) we have

$$[\varphi_n(\alpha)]^k \equiv \chi_k(\alpha)$$

for the eigenfunction for $e^{ikn\beta}$, $k = 0, \pm 1, \pm 2, \cdots$. The χ_k form a complete system in $L^2(\rho)$; this can be seen as follows: Assume that there exists an eigenvalue $m > n$ which is no multiple of n. Then m, n have a greatest common factor (m, n) smaller than n. But then there exist integer numbers μ, ν such that $\mu m + \nu n = (m, n)$. Hence $(\varphi_m)^\mu$, $(\varphi_n)^\nu$ would be eigenfunctions with the eigenvalue $(m, n) < n$ contradicting that n is the smallest such number.

Now, by an isometric mapping, $L^2(\rho(\alpha))$ can be mapped onto $L^2_{(0,2\pi)}(\alpha)$ by requiring that $\chi_k(\alpha)$ corresponds to $e^{ik\alpha}$, and in $L^2_{(0,2\pi)}(\alpha)$ we have $\alpha_\beta = \alpha + n\beta \pmod{2\pi}$; from $G(\beta + 2\pi) = G(\beta)$, we have $n = \pm 1, \pm 2, \cdots$. This accomplishes the proof.

4. APPLICATION TO A LOCAL, RELATIVISTIC FIELD

The statement presented in Sec. 2 and proved in Sec. 3 can be specified to a case considered in Ref. 1.

This can be accomplished by assuming Lorentz invariance, spectral condition and locality for the field as well as cyclicity of a vacuum state Ω. In addition, we specify the transformation of the field under the symmetry group $G(\beta)$ to be linear, i.e.,

$$\begin{aligned} G(\beta)A(x)G^+(\beta) &= e^{in\beta}A(x), \\ G(\beta)A^+(x)G^+(\beta) &= e^{-in\beta}A^+(x). \end{aligned} \tag{4}$$

Then we can omit the assumption in Sec. 2 that $\mathfrak{R}'$ is Abelian as superfluous; it follows from a theorem proved by Borchers.[6]

Due to (1) and (3) we have for

$$\mathfrak{H}_\Delta = \int_\Delta^\oplus I_\alpha \mathfrak{H} = \int_\Delta^\oplus \mathfrak{H}_\alpha (d\alpha)^{\frac{1}{2}},$$

$$\Omega_\Delta = \int_\Delta^\oplus I_\alpha \Omega = \int_\Delta^\oplus \Omega_\alpha,$$

and, if A_α denotes an operator in $\mathfrak{H}_\alpha$,[7]

$$A_\Delta(x) = \int_\Delta^\oplus A_\alpha(x)$$

the formulas

$$\begin{aligned} G(\beta)\mathfrak{H}_\Delta &= \mathfrak{H}_{\Delta+n\beta}, \\ G(\beta)\Omega_\Delta &= \Omega_{\Delta+n\beta}, \\ G(\beta)A_\Delta(x)G^+(\beta) &= e^{in\beta}A_{\Delta+n\beta}(x), \end{aligned}$$

respectively.[8] These formulas are analogous to those given in Ref. 1, Eqs. (2.1) and (2.2).

Notice that almost all spaces $\mathfrak{H}_\alpha$ are Hilbert spaces of infinite dimension if we exclude the uninteresting case that $\mathfrak{H}$ consists of vacuum states only. This can be shown as follows.[9]

The unitary representation $U(\Lambda, a)$ of the Lorentz group is contained in $\mathfrak{R}''$ as was shown by Borchers,[6] therefore it is also reduced by the decomposition of the Hilbert space. Since, on the other hand, Ω is invariant under $G(\beta)$, it follows that $G(\beta)$ commutes with $U(\Lambda, a)$. Since $\mathfrak{H}$ has states not invariant under the Lorentz group, there exists a finite interval Δ such that every $\mathfrak{H}_\alpha$ with $\alpha \in \Delta$ contains states noninvariant under $U(\Lambda, a)$ and therefore having infinite dimension. But then the same holds for every other subinterval. Assume that the latter is not true; then there is an interval Δ' of length smaller than Δ such that $\int_{\Delta'}^\oplus \mathfrak{H}_\alpha (d\alpha)^{\frac{1}{2}}$ contains only vacua. There exists a $\phi \in \int_\Delta^\oplus \mathfrak{H}_\alpha (d\alpha)^{\frac{1}{2}}$ which is not invariant under $U(\Lambda, a)$ and mapped by a certain $G(\beta)$ into $\phi' \in \int_{\Delta'} \mathfrak{H}_\alpha (d\alpha)^{\frac{1}{2}}$. Applying $U(\Lambda, a)$, we get

$$\begin{aligned} U(\Lambda, a)G(\beta)\phi &= U(\Lambda, a)\phi' = \phi' \\ &= G(\beta)U(\Lambda, a)\phi \end{aligned}$$

such that $U(\Lambda, a)\phi$ would be mapped by $G(\beta)$ onto ϕ' too. But this contradicts the unitarity of $G(\beta)$ (one-to-one mapping).

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[6] H. J. Borchers, Nuovo Cimento **24**, 214 (1962); see also Appendix 1 in Ref. 1.

[7] The decomposition can also be done for the unbounded field operators as follows from E. A. Nussbaum, Duke Math. J. **31**, 33 (1964).

[8] We can redefine $\beta \to \beta' = n\beta$; then the periodicity assumption reads $G'(\beta') = G'(\beta' + 2\pi n)$.

[9] This, as well as the measure-preserving property, proved in Sec. 3(D) could also be derived by applying a more general theorem; see J. Dixmier, *Les Algebres D'operateurs dans L'espace Hilbertien* (Gautheir-Villars, Paris, 1957), Chap. II, Sec. 6, Theorem 4. We thank Dr. H. Araki for this information.

Classification of Irreducible Unitary Representations of Compact Simple Lie Groups. I

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An irreducible unitary representation of any group belongs to one of the three Wigner classes, potentially real, pseudo-real, or complex. The irreducible unitary representations of all the compact simple Lie groups except those of the type E are hereby classified. The similar classification for the simple groups E_6, E_7, and E_8 is completed in the next paper.

1. INTRODUCTION

GIVEN a (finite-dimensional matrix) representation D of a group G, the complex conjugate D^* of D is also a representation of G. If D is irreducible and unitary, so is D^*. The irreducible unitary representations (IUR's) D and D^* may or may not be equivalent. If they are not equivalent, we say, following Wigner,[1] that D is complex. If, on the other hand, D and D^* are equivalent, i.e., if there exists a C, the same for all group elements, such that

$$D = CD^*C^{-1},$$

then it can be proved that the unitary matrix C is either symmetric or antisymmetric and there are two cases to be distinguished.

(1) C is symmetric: In this case a transformation matrix U can be found such that the representation $\rho = UDU^{-1}$ is real: $\rho = \rho^*$.

(2) C is antisymmetric: In this case no U with the above property exists. However, one can find a U such that the representation $\rho = UDU^{-1}$ satisfies the condition $Z\rho = \rho^* Z$, where Z is the real antisymmetric unitary matrix having nonzero elements only in the super- and subdiagonals:

$$Z = \begin{bmatrix} 0 & -1 & 0 & 0 & \cdots \\ 1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & -1 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix} \equiv \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \dotplus \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \dotplus \cdots. \quad (1.1)$$

We call Z the pseudo-unit matrix.

The above two properties are intrinsic to the representation and are not affected by further similarity transformations.

When D and D^* are equivalent, $D = CD^*C^{-1}$, D is said to be real. Furthermore, it is of the positive sign or "potentially real" if C is symmetric, $C^T = C$, and is of the negative sign or "pseudo-real" if C is antisymmetric, $C^T = -C$.

We examine in this article all the irreducible unitary representations of simple Lie groups except the three isolated ones E_6, E_7, and E_8 and determine its Wigner class whether it is complex or real and if real of what sign. The same question about the E_6, E_7, and E_8 will be answered in the next article.

2. ROOTS, WEIGHTS, AND CHARACTERIZATION OF THE REPRESENTATIONS

A unitary representation of a Lie group can be inferred from that of its algebra by exponentiation. For the algebra of order r and rank l we choose a Cartan–Weyl basis, so that the commutation relations assume the standard form[2]:

$$\begin{aligned} &[H_i, H_j] = 0, \qquad i, j = 1, 2, \cdots, l; \\ &[H_i, E_{\pm\alpha}] = \pm r_i(\alpha) E_{\pm\alpha}, \\ &\qquad\qquad \alpha = 1, 2, \cdots, \tfrac{1}{2}(r - l); \\ &[E_\alpha, E_{-\alpha}] = \sum_{i=1}^{l} r_i(\alpha) H_i; \qquad [E_\alpha, E_\beta] = N_{\alpha\beta} E_{\alpha+\beta}, \end{aligned} \quad (2.1)$$

$N_{\alpha\beta} \neq 0$ only if $\mathbf{r}(\alpha) + \mathbf{r}(\beta)$ is also a root. The Killing scalar products are

$$(H_i, H_j) = 1, \qquad (E_\alpha, E_{-\alpha}) = 1,$$

all other scalar products are zero.[2] The roots $\mathbf{r}(\alpha)$ satisfy the condition

$$\sum_\alpha r_i(\alpha) r_j(\alpha) = \delta_{ij} = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{otherwise,} \end{cases}$$

and the structure constants are real.[3]

$$r_i(\alpha) = r_i^*(\alpha), \qquad N_{\alpha\beta} = N_{\alpha\beta}^*. \quad (2.2)$$

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[1] E. P. Wigner, *Group Theory and Its Applications to the Quantum Mechanics of Atomic Spectra* (Academic Press Inc., New York, 1959), pp. 285–288. Professor Wigner has kindly pointed out that this classification is due originally to G. Frobenius and I. Schur, Proc. Berlin Acad. 186 (1906).

[2] E. Cartan, thesis (1894), reprinted in *Oeuvres Complètes* (Gauthier-Villars, Paris, 1952), Part 1, Vol. 1.

[3] H. Weyl, Math. Z. **23**, 271 (1925); *ibid.* **24**, 328 (1926).

A positive root is one whose first nonzero component is positive. A simple root is a positive root which cannot be written as a sum of two positive roots. There are l simple roots $\mathbf{s}_i$, $i = 1, \cdots, l$, and any other root $\mathbf{r}$ can be written as

$$\mathbf{r} = \sum_{i=1}^{l} a_i \mathbf{s}_i \tag{2.3}$$

with integers a_i, all of the same sign.[2,4]

The matrices representing E_α and $E_{-\alpha}$ will be Hermitian conjugates of each other and those representing H_i will be Hermitian and can be taken to be diagonal and hence real. Thus the coefficient of E_α must be the complex conjugate of that of $E_{-\alpha}$ and the coefficient of H_i must be real in the linear form to be exponentiated.

$$D(a, b) = \exp\{i \sum_j a_j H_j + i \sum_\alpha b_\alpha E_\alpha\}, \qquad a_j = a_j^*, \quad b_\alpha = b_{-\alpha}^*. \tag{2.4}$$

An irreducible representation can be characterized by its highest weight.[5] This highest-weight $\mathbf{M}$ can be written in terms of the l fundamental dominant weights $\mathbf{\Pi}_i$ as

$$\mathbf{M} = \sum_{i=1}^{l} \lambda_i \mathbf{\Pi}_i \tag{2.5}$$

with nonnegative integers λ_i. Thus an irreducible representation can be characterized by the l nonnegative integers λ_i once the fundamental dominant weights $\mathbf{\Pi}_i$ are known.

To get the fundamental dominant weights one may use the condition that for any weight $\mathbf{M}$ and any root $\mathbf{r}$, $2\mathbf{M}\cdot\mathbf{r}/\mathbf{r}\cdot\mathbf{r}$ is an integer. For each root $\mathbf{r}$ we get a linear condition on the components of $\mathbf{M}$. These conditions are linearly independent only for the simple roots, and when inverted to have the form of Eq. (2.5) give the fundamental dominant weights. In other words, the fundamental dominant-weight $\mathbf{\Pi}_i$ is defined by the equations

$$2\mathbf{\Pi}_i \cdot \mathbf{s}_j / \mathbf{s}_j \cdot \mathbf{s}_j = \delta_{ij} \tag{2.6}$$

for any simple root $\mathbf{s}_j$. We reproduce in the Appendix a possible choice of the roots and the fundamental dominant weights.

For any weight $\mathbf{M}$ and any root $\mathbf{r}$, one gets another weight by reflecting $\mathbf{M}$ in the plane perpendicular to $\mathbf{r}$

$$S_\mathbf{r}\mathbf{M} = \mathbf{M} - 2(\mathbf{M}\cdot\mathbf{r}/\mathbf{r}\cdot\mathbf{r})\mathbf{r}.$$

The reflections $S_\mathbf{r}$ together with their logical products form a (finite) group S, known as the Weyl group. If $2\mathbf{M}\cdot\mathbf{r}/\mathbf{r}\cdot\mathbf{r} \geq 2$, then $\mathbf{M} - j\mathbf{r}$ with $1 \leq j \leq 2\mathbf{M}\cdot\mathbf{r}/\mathbf{r}\cdot\mathbf{r}$, are also weights. Starting with the highest weight, one can construct all the weights of the IUR in this way.

Another important quantity relating to a representation is its character χ. It is defined[3,6] by

$$\chi(\lambda, \phi) = \xi(\lambda, \phi)/\xi(0, \phi), \qquad \xi(\lambda, \phi) = \sum_S \delta_S \exp[i(S\mathbf{K})\cdot\phi],$$

where the sum is over the Weyl group S of reflections defined above and δ_S is $+1$ for an even number of reflections and -1 for an odd number. Let $\mathbf{R}$ be the semi-sum over the positive roots

$$\mathbf{R} = \tfrac{1}{2} \sum_{\alpha,+} \mathbf{r}(\alpha),$$

then $\mathbf{K}$ is the sum of $\mathbf{R}$ and the highest weight $\mathbf{M}$ of the representation

$$\mathbf{K} = \mathbf{R} + \mathbf{M}(\lambda_1, \lambda_2, \cdots, \lambda_l) = \mathbf{R} + \sum_{i=1}^{l} \lambda_i \mathbf{\Pi}_i. \tag{2.7}$$

Two (finite-dimensional) representations are equivalent if and only if their characters are equal. Thus an IUR is real or complex according as its character is real or complex. This means that an IUR is real if and only if[7] one can find an element S_1 of the Weyl group S which changes the sign of $\mathbf{K}$:

$$S_1\mathbf{K} = -\mathbf{K}.$$

However, we have not been able to read out the sign of a real IUR from its character alone.

In dealing with the reduction of the direct product of two IUR's the formula for the dimension number is helpful. In terms of the highest-weight $\mathbf{M}$, the

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[4] E. B. Dynkin, Usp. Math. Nauk 59 (1947); Transl. Am. Math. Soc. No. 17 (1950).

[5] E. Cartan, Bull. Soc. Math. France 41, 53 (1913), reprinted in *Oeuvres Complètes*, Part 1, Vol. 1. In this article we noticed two serious errors in the enumeration of the multiplicities of various weights of the groups C_n and E_7. For the fundamental representations of the group C_n, the multiplicity of the weights of g_r which are obtained from reflections of the highest weight of $g_{r-2\alpha}$ is

$$\frac{(n-r+1)(n-r+2\alpha)!}{\alpha!\,(n-r+\alpha+1)!} \text{ and not } \frac{n!}{\alpha!\,(n-\alpha)!} - 1$$

as given by Cartan. Similarly, for the group E_7, the multiplicity of the weight $\mathbf{\Pi}_2$ in the representation g_6 is 71 and not 56. Cartan missed the 15 states $[x_{1i}y_jy_{ij}]$. Thanks are due Dr. P. K. Srivastava, who strongly doubted the number 56.

[6] R. E. Behrends, J. Dreitlein, C. Fronsdal, and B. W. Lee, Rev. Mod. Phys. 34, 1 (1962).

[7] H. Chandra, Ann. Math. 50, 68, 900 (1949); Proc. Am. Math. Soc. 1, 205 (1950).

dimension number of an IUR is given by[8]

$$N(\lambda_1, \lambda_2, \cdots, \lambda_l) = \prod_{\alpha,+} \left\{1 + \frac{\mathbf{M}\cdot\mathbf{r}(\alpha)}{\mathbf{R}\cdot\mathbf{r}(\alpha)}\right\}, \qquad (2.8)$$

where $\mathbf{R}$ is the semi-sum of the positive roots and the product is taken over all the positive roots.

Using the character formula of Weyl one can deduce that [9]

$$\sum_S \delta_S \gamma(\mathbf{m} + \mathbf{R} - S\mathbf{R}) = \delta_{mM} = \begin{cases} 1, & \text{if } \mathbf{m} = \mathbf{M}, \\ 0, & \text{otherwise}, \end{cases} \qquad (2.9)$$

where $\gamma(\mathbf{w})$ is the multiplicity of the weight $\mathbf{w}$, $\mathbf{M}$ is the highest weight of the IUR, $\mathbf{m}$ any other weight, and the summation is taken over all the reflections. In particular $\gamma(\mathbf{w}) = 0$, if $\mathbf{w}$ is not a weight. Equation (2.9) together with

$$\gamma(S\mathbf{m}) = \gamma(\mathbf{m}) \qquad (2.10)$$

is sufficient to determine the multiplicity of a weight $\mathbf{m}$, if the multiplicities of all the higher weights are known. The multiplicity of the highest weight being one, we can determine the multiplicities of all the weights step by step. (See note added in proof.)

Now the reduction process is quite straightforward.

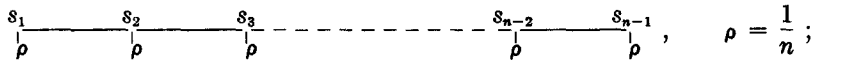
3. THE FUNDAMENTAL DOMINANT WEIGHTS

Since we need to know only the ratios of the various scalar products for the roots and weights, it is sometimes convenient to use the Dynkin diagram. This diagram consists in representing the simple roots by points, assigning to each point a number equal to the square of that root and joining two points by a single, double, or triple line according as the angle between the represented roots is 120°, 135°, or 150°. If the angle is 90°, the points are not joined at all. As the simple roots are linearly independent,[4] they can be chosen to form a basis in the root space or in the weight space. Thus a root $\mathbf{r}$ is represented by the coefficients a_i in Eq. (2.3). Similarly, any weight can be expressed as a linear form of the simple roots and represented by the corresponding coefficients. As the simple roots do not form an orthogonal basis, one has to be careful in the manipulations.

If one can choose a set of l mutually orthogonal roots, where l is the rank of the group, then the Weyl reflections with respect to these roots will change the sign of any vector and in particular that of $\mathbf{K} = \mathbf{R} + \mathbf{M}$. This will then be a sufficient condition for all the IUR's to be real.[10] For all the IUR's to be real, this condition is also necessary as we have been able, in every individual case, to locate such a set of orthogonal roots.

Following is a list of Dynkin diagrams and fundamental dominant weights for the simple groups A_n, B_n, C_n, D_n, G_2, and F_4. The roots can be easily constructed by Dynkin's method[4] and we do not find it useful to list them.

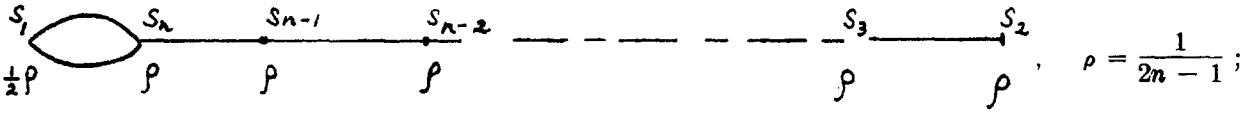
A_{n-1} or SU_n



$$\rho = \frac{1}{n};$$

$$\Pi_j = \frac{1}{n}\left\{\sum_{k=1}^{j} k(n-j)\mathbf{s}_k + \sum_{k=j+1}^{n-1} j(n-k)\mathbf{s}_k\right\}, \qquad j = 1, 2, \cdots, n-1.$$

B_n or 0_{2n+1}



$$\rho = \frac{1}{2n-1};$$

$$\Pi_1 = \tfrac{1}{2}n\mathbf{s}_1 + \frac{1}{2}\sum_{k=2}^{n}(k-1)\mathbf{s}_k,$$

$$\Pi_j = (j-1)\mathbf{s}_1 + \sum_{k=2}^{j}(k-1)\mathbf{s}_k + (j-1)\sum_{k=j+1}^{n}\mathbf{s}_k, \qquad j = 2, 3, \cdots, n.$$

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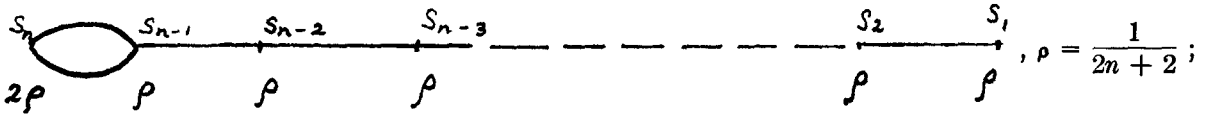
[8] H. Weyl, Ref. 3, p. 389.

[9] G. Racah, "Group Theoretical Concepts and Methods in Elementary Particle Physics," in *Istanbul Summer School Lectures, 1962*, F. Gursey, Ed. (Gordon and Breach Science Publishers, Inc., New York, London, 1962).

[10] I am thankful to Dr. P. K. Srivastava for pointing out that this was the case in all such constructions.

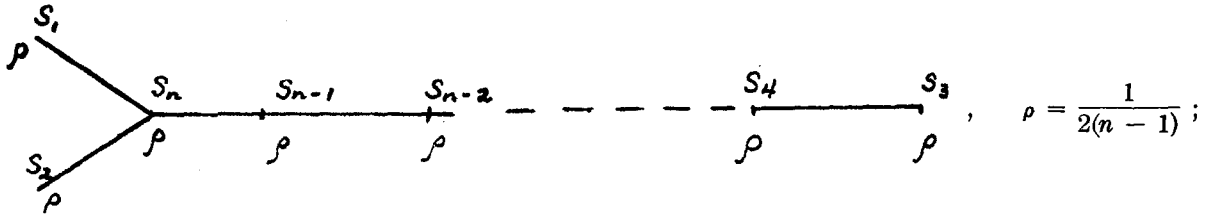
C_n or $Sp(n)$



$$\rho = \frac{1}{2n+2};$$

$$\Pi_j = \tfrac{1}{2}j s_n + \sum_{k=1}^{j} k s_k + j \sum_{k=j+1}^{n} s_k, \qquad j = 1, 2, \cdots, n.$$

D_n or 0_{2n}



$$\rho = \frac{1}{2(n-1)};$$

$$\Pi_1 = \tfrac{1}{4}n s_1 + \tfrac{1}{4}(n-2)s_2 + \tfrac{1}{2}\sum_{k=3}^{n}(k-2)s_k,$$

$$\Pi_2 = \tfrac{1}{4}(n-2)s_1 + \tfrac{1}{4}n s_2 + \frac{1}{2}\sum_{k=3}^{n}(k-2)s_k,$$

$$\Pi_j = \tfrac{1}{2}(j-2)(s_1+s_2) + \sum_{k=3}^{j}(k-2)s_k + (j-2)\sum_{k=j+1}^{n} s_k, \qquad j = 3, 4, \cdots, n.$$

G_2

$$\rho = \frac{1}{12};$$

$$\Pi_1 = 2s_1 + s_2, \qquad \Pi_2 = 3s_1 + 2s_2.$$

F_4

$$\rho = \frac{1}{18};$$

$$\Pi_1 = 2s_1 + 3s_3 + s_2 + 2s_4, \qquad \Pi_2 = 2s_1 + 4s_3 + 2s_2 + 3s_4,$$

$$\Pi_3 = 3s_1 + 6s_3 + 2s_2 + 4s_4, \qquad \Pi_4 = 4s_1 + 8s_3 + 3s_2 + 6s_4.$$

4. CLASSIFICATION OF THE IRREDUCIBLE UNITARY REPRESENTATIONS

The problem of classification is greatly reduced by the following few lemmas. In what follows, we are concerned with the finite-dimensional unitary irreducible representations.

Lemma 1: If on reducing the direct product of two real representations D_1 and D_2 one gets a real representation D_3 then the product of the signs of these three real representations D_1, D_2, and D_3 is positive.

Proof: Let the irreducible real representation D_3 occur in the reduction of the direct product of two irreducible real representations D_1 and D_2

$$D_1 = A_1 D_1^* A_1^{-1}, \qquad D_2 = A_2 D_2^* A_2^{-1}, \tag{4.1}$$

$$B(D_1 \times D_2)B^{-1} = D_3 + L, \qquad D_3 = A_3 D_3^* A_3^{-1},$$

where L in the direct sum above may be irreducible, further reducible, or even nonexistent. Then from the matrix equation

$$(P \times Q)(R \times S) = PR \times QS$$

we have

$$D_1 \times D_2 = (A_1 \times A_2)(D_1^* \times D_2^*)(A_1 \times A_2)^{-1},$$

or using Eq. (4.1)

$$D_3 \dotplus L = B(A_1 \times A_2)B^{*-1} \times (D_3^* \dotplus L^*)B^*(A_1 \times A_2)^{-1}B^{-1}.$$

Therefore, one may write

$$B(A_1 \times A_2)B^{*-1} = \begin{bmatrix} A_3 & \alpha \\ \beta & A_L \end{bmatrix},$$

where

$$L = A_L L^* A_L^{-1}.$$

Thus the symmetry of A_3 and A_L is the same as that of $A_1 \times A_2$. Also

$$(A_1 \times A_2)^T = A_1^T \times A_2^T,$$

and we have proved the lemma.

Lemma 2: If on reducing the direct product of a representation with (a representation equivalent to) its complex conjugate, a real representation appears, then its sign is positive.

Proof: Let a real IUR D_2 occur in the reduction of the direct product of D_1 and $A_1 D_1^* A_1^{-1}$ (equivalent to D_1^*),

$$B(D_1 \times A_1 D_1^* A_1^{-1})B^{-1} = D_2 \dotplus L,$$
$$D_2 = A_2 D_2^* A_2^{-1},$$

so that

$$(1 \times A_1)(D_1 \times D_1^*)(1 \times A_1)^{-1} = B^{-1}(D_2 \dotplus L)B, \qquad (4.2)$$

where 1 is the unit matrix. Taking the complex conjugate and using the fact that $R \times S$ and $S \times R$ are related by a similarity transformation, we have

$$(1 \times A_1)^* P (D_1 \times D_1^*) P^{-1} (1 \times A_1)^{*-1} = B^{*-1}(D_2^* \dotplus L^*)B^*,$$

where

$$P(D_1 \times D_1^*)P^{-1} = D_1^* \times D_1. \qquad (4.3)$$

Using Eq. (4.2) once more one deduces that

$$D_2 \dotplus L = N(D_2^* \dotplus L^*)N^{-1},$$

where

$$N = B(1 \times A_1)P^{-1}(1 \times A_1)^T B^T = \begin{bmatrix} A_2 & \alpha \\ \beta & A_L \end{bmatrix}. \qquad (4.4)$$

The matrix N is symmetric if P is so. Now for any R and S, the relation

$$P(R \times S) = (S \times R)P$$

is satisfied by the choice

$$P_{ij,kl} = \delta_{il}\,\delta_{jk}.$$

This P is nonsingular and symmetric if the dimensions of the square matrices R and S are equal. As the dimensions of D_1 and D_1^* are the same, the P occurring in Eqs. (4.3) and (4.4) is symmetric and unitary. Hence A_2 is symmetric and D_2 is positive.

Lemma 3: The unitary matrix C transforming a real representation D of the group into its complex conjugate D^*:

$$CDC^{-1} = D^*$$

will transform the representation L of the corresponding algebra into $-L^T$

$$CLC^{-1} = -L^T \quad \text{or} \quad CL = -L^T C$$

and conversely any C transforming L to $-L^T$ will transform D to D^*.

Moreover, the only nonzero elements of C will be those connecting the states of equal and opposite weights.

Proof: From the relation

$$D(\phi) = \exp(iL \cdot \phi)$$

the first part of the lemma is obvious. For the last part one may consider the equation

$$CH_i + H_i C = 0,$$

where H_i diagonal and real; and the diagonal elements of H_i are the jth component of the weights of the various states.

Lemma 4: If the dimension number of a real IUR is odd, then its sign is positive.

This is obvious from the fact that an antisymmetric unitary (transformation) matrix C of odd-dimension number does not exist.

Lemma 5: The regular representation is positive real.

This result is the same as Eq. (2.2) above.

In the light of the above lemmas let us examine the IUR's of simple Lie groups one by one.

4.1. The Group A_{n-1} or SU_n

The set of reflections corresponding to the roots $\sum_{i=j}^{n-j} \mathbf{s}_i$ for $j = 1, 2, \cdots, [\frac{1}{2}n] + 1$, where $[\frac{1}{2}n]$ is the largest integer less than or equal to $\frac{1}{2}n$, when ap-

plied in any order to the vector $\sum_1^{n-1} a_i \mathbf{s}_i$ changes it to $-\sum_1^{n-1} a_{n-i}\mathbf{s}_i$ for arbitrary coefficients a_i. Thus the above set of reflections changes $\mathbf{K}_i = \mathbf{R} + \mathbf{\Pi}_i$ to $-\mathbf{K}_{n-i} = -(\mathbf{\Pi}_{n-i} + \mathbf{R})$ for $i = 1, 2, \cdots, n-1$, where $\mathbf{R}$ is the semi-sum over the positive roots:

$$\mathbf{R} = \frac{1}{2}\sum_{i=1}^{n-1} j(n-j)(\mathbf{s}_i + \mathbf{s}_{n-j}).$$

Therefore the character χ_i of the fundamental representation g_i corresponding to the dominant weight $\mathbf{\Pi}_i$ is the complex conjugate of that of g_{n-i} corresponding to $\mathbf{\Pi}_{n-i}$. Thus an IUR $(\lambda_1, \lambda_2, \cdots, \lambda_{n-1})$ is real if an only if $\lambda_i = \lambda_{n-i}$ for $i = 1, 2, \cdots, n-1$. If n is odd, none of the fundamental representations is real and all real representations arise on reduction of direct products of mutually complex conjugate representations. Hence all of them have positive sign. If n is even, $n = 2m$, one of the fundamental representations, i.e., the g_m corresponding to $\mathbf{\Pi}_m$ is real and we show below by an explicit construction of the transformation matrix C that this representation has the sign $(-1)^m$.

The representation g_m of SU_{2m} having the highest-weight $\mathbf{\Pi}_m$ is $({}^{2m}C_m)$-dimensional and indicates how the ${}^{2m}C_1$ representation g_1 of the SU_{2m} itself transforms the antisymmetric quantities $[x_{\alpha_1}x_{\alpha_2}\cdots x_{\alpha_m}]$; $\alpha_1 < \alpha_2 < \cdots < \alpha_m$; $\alpha_1, \alpha_2, \cdots, \alpha_m = 1, 2, \cdots, 2m$; into themselves. As the trace of any H_i is zero, we see from Lemma 3 that the only nonzero elements of C are those connecting the states $(\alpha_1\,\alpha_2\cdots\alpha_m)$ and $(\beta_1\beta_2\cdots\beta_m)$, where $\alpha_1 < \alpha_2 < \cdots < \alpha_m$, $\beta_1 < \beta_2 < \cdots < \beta_m$ and $\alpha_1\cdots\alpha_m\beta_1\cdots\beta_m$ are the indices $1, 2, \cdots, 2m$ in some order. Next, a consideration of the equation

$$CE_{(ik)} = -E_{(ik)}^T C$$

tells us that the nonzero elements of C all have the same magnitude and may differ only in the sign. This sign depends on the order of the indices and is easily determined. Thus C may be taken to be

$$C_{(\alpha_1\cdots\alpha_m),(\beta_1\cdots\beta_m)} = (-1)^\epsilon,$$

where $\alpha_1 < \cdots < \alpha_m$, $\beta_1 < \cdots < \beta_m$, ϵ is the parity of the permutation

$$\begin{pmatrix} 1\,2\cdots m, & m+1\cdots 2m \\ \alpha_1\,\alpha_2\cdots\alpha_m & \beta_1\cdots\beta_m \end{pmatrix},$$

and all other elements of C are zero.

This C clearly satisfies the equation

$$C^T = (-1)^m C$$

and therefore the sign of the real representation ${}^{2m}C_m$ or g_m of SU_{2m} having the highest weight $\mathbf{\Pi}_m$ is $(-1)^m$.

The final result for the group A_{n-1} can therefore be stated as follows.

Theorem 1: The representation $(\lambda_1, \lambda_2, \cdots, \lambda_{n-1})$ of A_{n-1} is complex, unless $\lambda_i = \lambda_{n-i}$, $i = 1, 2, \cdots, n-1$, in which case it is real. The sign is plus if n is odd, and $(-1)^{m\lambda_m}$ if n is even, $n = 2m$, m an integer.

4.2. The Group B_n or 0_{2n+1}

The n roots $\mathbf{s}_1$, $\mathbf{s}_1 + \sum_{j=k}^n \mathbf{s}_j$, $k = 2, 3, \cdots, n$ form an orthogonal system. The corresponding reflections will change the sign of any vector and in particular that of $\mathbf{K} = \mathbf{R} + \mathbf{M}$. Thus all the IUR's of B_n are real. To determine the sign, it is sufficient, in view of the Lemma 1, to determine the signs of the fundamental representations only.

The representation g_2 having the highest weight $\mathbf{\Pi}_2$ is the well-known set of $(2n+1) \times (2n+1)$ orthogonal matrices leaving the symmetric bilinear form $x_0^2 + \sum_{i=1}^n (x_i^2 + x_{-i}^2)$ invariant. The infinitesimal matrix

$$\sum a_i H_i + \sum (b_\alpha E_\alpha + b_\alpha^* E_{-\alpha})$$

is antisymmetric as well as Hermitian and hence is pure imaginary. The matrix C in $CL = -L^T C$ is therefore the unit matrix. The representation g_2 is real positive.

One can derive the above result also as follows. The matrices D of the representation g_2 satisfy $D^T D = 1$. They are also unitary $D^+ D = 1$. Therefore they are already real: $D = D^*$.

The representations $g_3, g_4, \cdots, g_n$ having the highest weights $\mathbf{\Pi}_3, \mathbf{\Pi}_4, \cdots, \mathbf{\Pi}_n$ arise on reducing the direct powers of g_2. All these representations are therefore real positive according to Lemma 1.

The representation g_1 having the highest-weight $\mathbf{\Pi}_1$ remains to be examined. This representation is given by[5]

$$H_i = \tfrac{1}{2}\sum \epsilon_i x_{\epsilon_1\cdots\epsilon_n} p_{\epsilon_1\cdots\epsilon_n}, \tag{4.5}$$

$$E_{(+j)} = \sum \epsilon_1\cdots\epsilon_{j-1} x_{\epsilon_1\cdots\epsilon_{j-1}+1\epsilon_{j+1}\cdots\epsilon_n} \times p_{\epsilon_1\cdots\epsilon_{j-1}-1\epsilon_{j+1}\cdots\epsilon_n}$$

$$E_{(-j)} = E_{(+j)}^+, \tag{4.5'}$$

$$E_{(+j+k)} = \sum \epsilon_{j+1}\cdots\epsilon_{k-1} \times x_{\epsilon_1\cdots\epsilon_{j-1}+1\epsilon_{j+1}\cdots\epsilon_{k-1}+1\epsilon_{k+1}\cdots\epsilon_n} \times p_{\epsilon_1\cdots\epsilon_{j-1}-1\epsilon_{j+1}\cdots\epsilon_{k-1}-1\epsilon_{k+1}\cdots\epsilon_n} \tag{4.6}$$

$$E_{(+j-k)} = \sum \epsilon_{j+1} \cdots \epsilon_{k-1} \times x_{\epsilon_1 \cdots \epsilon_{j-1}+1\epsilon_{j+1}\cdots\epsilon_{k-1}-1\epsilon_{k+1}\cdots\epsilon_n'} \times p_{\epsilon_1\cdots\epsilon_{j-1}-1\epsilon_{j+1}\cdots\epsilon_{k-1}+1\epsilon_{k+1}\cdots\epsilon_n}, \quad (4.7)$$

$$E_{(-j-k)} = E^+_{(+j+k)}, \qquad E_{(-j+k)} = E^+_{(+j-k)}, \qquad 1 \le j < k \le n, \quad (4.8)$$

in terms of the basis states $x_{\epsilon_1\cdots\epsilon_n}$ where the indices ϵ are $+1$ or -1 independently of each other. Putting $\epsilon_j' = -\epsilon_j$ we see from the equation $CL = -L^TC$, with L equal to H_j or $E_{(+j)}$ that the nonzero elements of the matrix C (between the states $x_{\epsilon_1\cdots\epsilon_n}$ and $x_{\epsilon_1'\cdots\epsilon_n'}$) satisfy the relation

$$C_{(\epsilon_1\cdots\epsilon_{j-1}\epsilon_j'\epsilon_{j+1}\cdots\epsilon_n),(\epsilon_1'\cdots\epsilon_{j-1}'\epsilon_j\epsilon_{j+1}'\cdots\epsilon_n')} = (-1)^i C_{(\epsilon_1\cdots\epsilon_n),(\epsilon_1'\cdots\epsilon_n')}.$$

Hence one concludes that

$$C^T = (-1)^{1+2+\cdots+n}C = (-1)^{\frac{1}{2}n(n+1)}C$$

and the sign of g_1 is $(-1)^{\frac{1}{2}n(n+1)}$.

For the group B_n we therefore have the following result

Theorem 2: All the IUR's of B_n are real. The sign of the representation $(\lambda_1, \cdots, \lambda_n)$ is $(-1)^{\frac{1}{2}n(n+1)\lambda_1}$.

4.3. The Group C_n or $Sp(n)$

The n roots $\mathbf{s}_n$, $\mathbf{s}_n + 2\sum_{j=k}^{n-1}\mathbf{s}_j$, $j = 1, 2, \cdots, n-1$ form an orthogonal system. Hence (by the remark of Sec. 3) all the IUR's of C_n are real.

The representation g_1 is the well-known set of $2n \times 2n$ symplectic matrices leaving the antisymmetric bilinear form $\sum_{i=1}^{n}(x_iy_{-i} - x_{-i}y_i)$ invariant. The matrices D of g_1 satisfy the relation $D^TZD = Z$, where Z is pseudo-unit matrix of Eq. (1.1). The matrices D are also unitary: $D^\dagger D = 1$. So that after a little manipulation $D = Z^{-1}D^*Z$ and Z is antisymmetric. Thus g_1 is real negative.

The representations g_2, g_3, $\cdots$, g_n are obtained by the reduction of the successive direct powers of g_1, hence they alternate in sign.

Theorem 3: The IUR $(\lambda_1, \cdots, \lambda_n)$ of C_n is real and has the sign $(-1)^{\lambda_1+\lambda_3+\lambda_5+\cdots}$.

4.4. The Group D_n or 0_{2n}

By an argument similar to that used for B_n, the fundamental representations g_3, g_4, $\cdots$, g_n of D_n are positive real. There remains to examine only the representations g_1 and g_2.

Let n be odd, $n = 2m + 1$. Then the reflections corresponding to the roots $\mathbf{s}_{2j+1}$, $\mathbf{s}_1 + \mathbf{s}_2 + \mathbf{s}_{2j+1} + 2\sum_{i=2j+2}^{n}\mathbf{s}_i$, for $j = 1, 2, \cdots, m$ change $\mathbf{K}_1 = \mathbf{R} + \mathbf{\Pi}_1$ to $-\mathbf{K}_2 = -(\mathbf{R} + \mathbf{\Pi}_2)$ and $\mathbf{K}_2$ to $-\mathbf{K}_1$. The representations g_1 and g_2 are therefore (equivalent to) the complex conjugates of each other if n is odd. Next let n be even, $n = 2m$. Then the $n = 2m$ roots $\mathbf{s}_1$, $\mathbf{s}_2$, $\mathbf{s}_{2j+1}$, $\mathbf{s}_1 + \mathbf{s}_2 + \mathbf{s}_{2j+1} + 2\sum_{i=2j+2}^{n}\mathbf{s}_i$, $j = 1, 2, \cdots, m-1$, form an orthogonal system and all the IUR's are therefore real (Sec. 3).

One must still examine the signs of g_1 and g_2 in case n is even. These representations are given by Eqs. (4.5)–(4.8) with the restriction that the product of all the ϵ is $+1$ for g_1 and -1 for g_2. It is now a trivial matter to verify that either for g_1 or for g_2 the transformation matrix C satisfies the relation

$$C_{(\epsilon_1\cdots\epsilon_{2j-2}\epsilon_{2j-1}'\epsilon_{2j}'\epsilon_{2j+1}\cdots\epsilon_n),(\epsilon_1'\cdots\epsilon_{2j-2}'\epsilon_{2j-1}\epsilon_{2j}\epsilon_{2j+1}'\cdots\epsilon_n')} = -C_{(\epsilon_1\cdots\epsilon_n),(\epsilon_1'\cdots\epsilon_n')}.$$

Therefore, $C^T = (-1)^{\frac{1}{2}n}C$, n even. The conclusion is as follows.

Theorem 4: The IUR $(\lambda_1, \lambda_2, \cdots, \lambda_n)$ of D_n is complex only when n is odd and $\lambda_1 \neq \lambda_2$. In all other cases it is real. The sign is $(-1)^{\lambda_1+\lambda_2}$ if $n = 4m + 2$, m an integer. In all other real cases the sign is positive.

4.5. The Group G_2

Roots $\mathbf{s}_2$ and $2\mathbf{s}_1 + \mathbf{s}_2$ are orthogonal. Therefore all IUR's are real.

The representation g_1 is seven-dimensional; its sign is therefore positive (Lemma 4).

The 14-dimensional representation g_2 is the regular representation, and is therefore real positive (Lemma 5).

Theorem 5: All IUR's of G_2 are real positive.

4.6. The Group F_4

The four roots $\mathbf{s}_3$, $\mathbf{s}_3 + \mathbf{s}_4$, $\mathbf{s}_2 + \mathbf{s}_3 + \mathbf{s}_4$, and $2\mathbf{s}_1 + \mathbf{s}_2 + 3\mathbf{s}_3 + 2\mathbf{s}_4$ form an orthogonal system. Reflections corresponding to them change the sign of $\mathbf{K}$. All IUR's of F_4 are therefore real.

The direct product $g_1 \times g_1$ when reduced contains[5] the direct sum $g_1 + g_2 + g_3$. And the direct product $g_2 \times g_2$ on reduction gives,[5] apart from other things, a g_4. Thus all the representations have a positive sign. The signs of g_2 (regular) and g_3 (odd-dimensional) could have been inferred directly as well.

Theorem 6: All IUR's of F_4 are real positive.

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APPENDIX

The roots and fundamental dominant weights of simple Lie algebras with a possible choice of an orthonormal basis.

A_{n-1} or SU_n

Elements of the algebra:

$$H_j = (2nj(j+1))^{-\frac{1}{2}}(e_{11} + \cdots + e_{jj} - je_{j+1,j+1}),$$

$$E_{+(ij)} = (2n)^{-\frac{1}{2}}e_{ij}, \qquad E_{-(ij)} = (2n)^{-\frac{1}{2}}e_{ji}, \qquad i < j,$$

with

$$e_{ij} = x_i p_j \equiv x_i \frac{d}{dx_j}; \qquad i, j = 1, 2, \cdots, n.$$

Roots:

$$\pm\alpha(jk) = \pm\frac{1}{(2n)^{\frac{1}{2}}}\left\{-\left(\frac{j-1}{j}\right)^{\frac{1}{2}}v_{j-1} + \left(\frac{k}{k-1}\right)^{\frac{1}{2}}v_{k-1} + \sum_{i=j}^{k-2}\frac{v_i}{[i(i+1)]^{\frac{1}{2}}}\right\}, \qquad 1 \le j < k \le n,$$

where v_i is a unit vector in the direction of the jth axis.

Simple roots:

$$\alpha(1n), \ -\alpha(j, j+1), \quad j = n-1, n-2, \cdots, 3, 2.$$

Fundamental dominant weights:

$$\mathbf{\Pi}_i = (2n)^{-\frac{1}{2}}\left\{\sum_{k=1}^{n-j}[k(k+1)]^{-\frac{1}{2}}v_k - \sum_{k=n-j+1}^{n-1}(n-j)[k(k+1)]^{-\frac{1}{2}}v_k\right\}.$$

The summations in the above are to be dropped whenever the corresponding indices do not exist. The fundamental representations $g_1, g_2, \cdots, g_{n-1}$ having $\mathbf{\Pi}_1, \mathbf{\Pi}_2, \cdots, \mathbf{\Pi}_{n-1}$ as their highest weights are usually denoted by the physicists as ${}^nC_1, {}^nC_2, \cdots, {}^nC_{n-2} = {}^nC_2^*$ and ${}^nC_{n-1} = {}^nC_1^*$, respectively. These numbers denote the dimensions.

Order of the Weyl group: $n!$.

B_n or O_{2n+1}

Elements of the algebra:

$$H_i = \frac{-i}{[2(2n-1)]^{\frac{1}{2}}}e'_{2i-1,2i},$$

$$E_{\pm i} = \frac{i}{[4(2n-1)]^{\frac{1}{2}}}\{e'_{2i-1,2n+1} \pm ie'_{2i,2n+1}\},$$

$$E_{\pm i\pm k} = \frac{i}{[8(2n-1)]^{\frac{1}{2}}}\{e'_{2i-1,2k-1} - e'_{2i,2k} \pm i(e'_{2i-1,2k} + e'_{2i,2k-1})\},$$

$$E_{\pm i\mp k} = \frac{i}{[8(2n-1)]^{\frac{1}{2}}}\{e'_{2i-1,2k-1} + e'_{2i,2k} \mp i(e'_{2i-1,2k} - e'_{2i,2k-1})\},$$

$$e'_{ik} = e_{ik} - e_{ki} = x_i p_k - x_k p_i.$$

Roots:

$$\alpha(\pm j) = \pm[2(2n-1)]^{-\frac{1}{2}}v_j,$$

$$\alpha(\pm j \pm k) = \pm[2(2n-1)]^{-\frac{1}{2}}(v_j + v_k),$$

$$\alpha(\pm j \mp k) = \pm[2(2n-1)]^{-\frac{1}{2}}(v_j - v_k).$$

Simple roots:

$$\alpha(n), \qquad \alpha(j-1, -j), \qquad j = 2, 3, \cdots, n.$$

Fundamental dominant weights:

$$\mathbf{\Pi}_1 = [2(2n-1)]^{-\frac{1}{2}}\cdot\tfrac{1}{2}(v_1 + \cdots + v_n),$$

$$\mathbf{\Pi}_j = [2(2n-1)]^{-\frac{1}{2}}(v_1 + \cdots + v_{j-1}), \qquad j = 2, 3, \cdots, n.$$

Dimensions of the fundamental representations:

$$2^n, \frac{(2n+1)!}{j!\,(2n-j+1)!} = {}^{2n+1}C_j, \qquad j = 1, 2, \cdots, n-1.$$

Order of the Weyl group: $2^n n!$.

C_n or $Sp(n)$

Elements of the algebra:

$$H_i = \frac{1}{2(n+1)^{\frac{1}{2}}}(e_{2i-1,2i-1} - e_{2i,2i}),$$

$$E_{+i} = (2n+2)^{-\frac{1}{2}}e_{2i-1,2i},$$

$$E_{-i} = (2n+2)^{-\frac{1}{2}}e_{2i,2i-1},$$

$$E_{+i+k} = \tfrac{1}{2}(n+1)^{-\frac{1}{2}}(e_{2i-1,2k} + e_{2k-1,2i}),$$

$$E_{-i-k} = \tfrac{1}{2}(n+1)^{-\frac{1}{2}}(e_{2i,2k-1} + e_{2k,2i-1}),$$

$$E_{+i-k} = \frac{i}{2}(n+1)^{-\frac{1}{2}}(e_{2i-1,2k-1} - e_{2k,2i}),$$

$$E_{-i+k} = \frac{i}{2}(n+1)^{-\frac{1}{2}}(e_{2i,2k} - e_{2k-1,2i-1}).$$

Roots:

$$\alpha(\pm j) = \pm\tfrac{1}{2}(n+1)^{-\frac{1}{2}}\cdot 2v_j,$$

$$\alpha(\pm j \pm k) = \pm\tfrac{1}{2}(n+1)^{-\frac{1}{2}}(v_j + v_k),$$

$$\alpha(\pm j \mp k) = \pm\tfrac{1}{2}(n+1)^{-\frac{1}{2}}(v_j - v_k).$$

Simple roots:

$\alpha(j-1,-j), \quad j=2,3,\cdots,n, \quad$ and $\quad \alpha(n)$.

Fundamental dominant weights:

$$\mathbf{\Pi}_i = \tfrac{1}{2}(n+1)^{-\frac{1}{2}}(v_1+\cdots+v_i), \quad j=1,2,\cdots,n.$$

Dimensions of the fundamental representations:

$$\frac{(2n+1)!\,(2n+2-2j)}{j!\,(2n+2-j)!}, \quad j=1,2,\cdots,n.$$

Order of the Weyl group: $2^n n!$.

D_n or 0_{2n}

Elements of the algebra:

$$H_i = -\frac{i}{2}(n-1)^{-\frac{1}{2}} e'_{2i-1,2i},$$

$$E_{\pm j\pm k} = \frac{i}{4}(n-1)^{-\frac{1}{2}}\{e'_{2j-1,2k-1} - e'_{2j,2k} \pm i(e'_{2j-1,2k} + e'_{2j,2k-1})\},$$

$$E_{\pm j\mp k} = \frac{i}{4}(n-1)^{-\frac{1}{2}}\{e'_{2j-1,2k-1} + e'_{2j,2k} \mp i(e'_{2j-1,2k} - e'_{2j,2k-1})\}.$$

Roots:

$$\alpha(\pm j \pm k) = \pm\tfrac{1}{2}(n-1)^{-\frac{1}{2}}(v_j+v_k),$$

$$\alpha(\pm j \mp k) = \pm\tfrac{1}{2}(n-1)^{-\frac{1}{2}}(v_j-v_k).$$

Simple roots:

$$\alpha(n-1,n), \quad \alpha(j-1,-j), \quad j=n,2,3,\cdots,n-1.$$

Fundamental dominant weights:

$$\mathbf{\Pi}_1 = \tfrac{1}{2}(n-1)^{-\frac{1}{2}}\cdot\tfrac{1}{2}(v_1+\cdots+v_{n-1}+v_n),$$

$$\mathbf{\Pi}_2 = \tfrac{1}{2}(n-1)^{-\frac{1}{2}}\cdot\tfrac{1}{2}(v_1+\cdots+v_{n-1}-v_n),$$

$$\mathbf{\Pi}_j = \tfrac{1}{2}(n-1)^{-\frac{1}{2}}(v_1+\cdots+v_{j-2}), \quad j=3,4,\cdots,n.$$

Dimensions of the fundamental representations:

$$2^{n-1},\ 2^{n-1},\ \frac{(2n)!}{j!\,(2n-j)!} = {}^{2n}C_j, \quad j=1,2,\cdots,n-2.$$

Order of the Weyl group: $2^{n-1}n!$.

G_2

Elements of the algebra:

$$H_1, H_2, E_{\pm\alpha}, \quad \alpha=1,2,\cdots,6.$$

Roots:

$$\mathbf{s}_1 = \frac{1}{4}\left(\frac{1}{\sqrt{3}}v_1 - v_2\right), \quad \mathbf{s}_2 = \tfrac{1}{2}v_2,$$

$$\mathbf{s}_1+\mathbf{s}_2,\ 2\mathbf{s}_1+\mathbf{s}_2,\ 3\mathbf{s}_1+\mathbf{s}_2,\ 3\mathbf{s}_1+2\mathbf{s}_2.$$

The first two roots are simple.

Fundamental dominant weights:

$$\mathbf{\Pi}_1 = (1/2\sqrt{3})v_1, \quad \mathbf{\Pi}_2 = \tfrac{1}{4}(\sqrt{3}\,v_1+v_2).$$

Dimensions of the fundamental representations: 7, 14.

Order of the Weyl group: 12.

F_4

There are 4 H and 48 E, a total of 52 elements.

Roots:

$$\pm\frac{1}{3\sqrt{2}}v_i, \quad \frac{1}{3\sqrt{2}}(\pm v_i \pm v_j),$$

$$\frac{1}{6\sqrt{2}}(\pm v_1 \pm v_2 \pm v_3 \pm v_4),$$

$i, j = 1, 2, 3, 4$; any sign combination.

Simple roots:

$$\mathbf{s}_1 = \frac{1}{6\sqrt{2}}(v_1-v_2-v_3-v_4), \quad \mathbf{s}_2 = \frac{1}{3\sqrt{2}}(v_2-v_3),$$

$$\mathbf{s}_3 = \frac{1}{3\sqrt{2}}v_4, \quad \mathbf{s}_4 = \frac{1}{3\sqrt{2}}(v_3-v_4).$$

Fundamental dominant weights:

$$\mathbf{\Pi}_1 = \frac{1}{3\sqrt{2}}v_1, \quad \mathbf{\Pi}_2 = \frac{1}{3\sqrt{2}}(v_1+v_2),$$

$$\mathbf{\Pi}_3 = \frac{1}{6\sqrt{2}}(3v_1+v_2+v_3+v_4),$$

$$\mathbf{\Pi}_4 = \frac{1}{3\sqrt{2}}(2v_1+v_2+v_3).$$

Dimensions of the fundamental representations: 26, 52, 273, 1274.

Order of the Weyl group: 1152.

Note added in proof: The method given in Sec. 2 for finding the multiplicities of various weights involves a summation over the Weyl group of reflections and therefore it is very long. Dr. P. K. Srivastava noticed and pointed out to the author a formula due to Freudenthal which involves a summation only over a few linear chains of weights. [See N. Jacobson, *Lie Algebras* (Interscience Publishers, Inc., New York, 1962), p. 247, Eq. 22.] It is much quicker to get the multiplicities by using this formula which reads as follows:

$$\{(\mathbf{M}+\mathbf{R})^2 - (\mathbf{m}+\mathbf{R})^2\}\gamma(\mathbf{m}) = 2\sum_{\substack{k=1\\ \alpha>0}}^{\infty}\{(\mathbf{m}+k\boldsymbol{\alpha})\cdot\boldsymbol{\alpha}\}\gamma(\mathbf{m}+k\boldsymbol{\alpha}).$$

Classification of Irreducible Unitary Representations of Compact Simple Lie Groups. II

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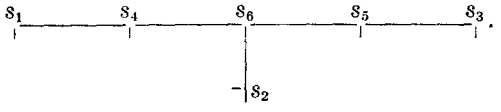
In continuation to a previous article, the classification of the irreducible unitary representations of the groups E_6, E_7, and E_8 into complex, potentially real, and pseudoreal catagories is completed.

1. INTRODUCTION

THIS is a continuation to an article by one of the authors[1]; a few lemmas from the first article will often be referred to. In Ref. 1 the irreducible unitary representations (IUR's) of the simple groups A_n, B_n, C_n, D_n, G_2, and F_4 were examined as to whether they were complex potentially real (real positive) or pseudo-real (real negative). Here the same thing is done for the remaining simple Lie groups E_6, E_7, and E_8.

2. THE GROUP E_6

The algebra is of rank 6 and order 78. The Dynkin diagram is



In labeling the roots, we have adopted, as always, the notation of Cartan. The fundamental dominant weights, determined by the equations

$$2\mathbf{\Pi}_i\cdot\mathbf{s}_j = (\mathbf{s}_j\cdot\mathbf{s}_j)\,\delta_{ij}$$

are

$$\mathbf{\Pi}_1 = \tfrac{1}{3}\begin{pmatrix}4&5&6&4&2\\&&3&&\end{pmatrix} \equiv \tfrac{1}{3}(4\mathbf{s}_1 + 5\mathbf{s}_4 + 6\mathbf{s}_6 + 4\mathbf{s}_5 + 2\mathbf{s}_3 + 3\mathbf{s}_2),$$

$$\mathbf{\Pi}_2 = \begin{pmatrix}1&2&3&2&1\\&&2&&\end{pmatrix},$$

$$\mathbf{\Pi}_3 = \tfrac{1}{3}\begin{pmatrix}2&4&6&5&4\\&&3&&\end{pmatrix}, \qquad \mathbf{\Pi}_4 = \tfrac{1}{3}\begin{pmatrix}5&10&12&8&4\\&&6&&\end{pmatrix},$$

$$\mathbf{\Pi}_5 = \tfrac{1}{3}\begin{pmatrix}4&8&12&10&5\\&&6&&\end{pmatrix}, \qquad \mathbf{\Pi}_6 = \begin{pmatrix}2&4&6&4&2\\&&3&&\end{pmatrix}. \tag{2.1}$$

The corresponding IUR's are denoted by g_1, g_2, $\cdots$, g_6. The sum of the fundamental dominant weights is $\mathbf{R}$, the semi-sum over the positive roots is

$$\mathbf{R} = \tfrac{1}{2}\sum_{\alpha,+}\mathbf{r}(\alpha) = \sum_{j=1}^{6}\mathbf{\Pi}_j = \begin{pmatrix}8&15&21&15&8\\&&11&&\end{pmatrix}. \tag{2.2}$$

The four roots

$$\begin{pmatrix}1&1&1&1&1\\&&0&&\end{pmatrix}, \begin{pmatrix}0&1&1&1&0\\&&0&&\end{pmatrix}, \begin{pmatrix}0&0&1&0&0\\&&0&&\end{pmatrix}, \text{ and } \begin{pmatrix}1&2&3&2&1\\&&2&&\end{pmatrix}$$

form an orthogonal set. Reflections corresponding to them change $\mathbf{K}_1 = \mathbf{\Pi}_1 + \mathbf{R}$ and $\mathbf{K}_4 = \mathbf{\Pi}_4 + \mathbf{R}$ to $-\mathbf{K}_3 = -(\mathbf{\Pi}_3 + \mathbf{R})$ and $-\mathbf{K}_5 = -(\mathbf{\Pi}_5 + \mathbf{R})$, respectively. The same set of reflections changes the signs of $\mathbf{K}_2 = \mathbf{\Pi}_2 + \mathbf{R}$ and $\mathbf{K}_6 = (\mathbf{\Pi}_6 + \mathbf{R})$. Hence the IUR's g_1 and g_4 are (equivalent to) the complex conjugates of g_3 and g_5, respectively, and the IUR's g_2 and g_6 are real.

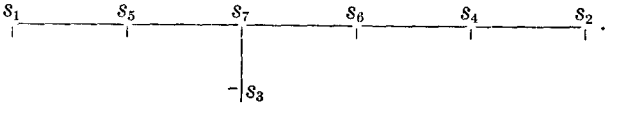
The IUR g_2 is the regular representation having 78 dimensions and the IUR g_6 has the dimension-number 2925, an odd number. Thus the real IUR's g_2 and g_6 are both positive.

From the above discussion follows the theorem

Theorem 7: The IUR of the group E_6 having the highest-weight $\sum \lambda_i\mathbf{\Pi}_i$ is real positive if $\lambda_1 = \lambda_3$ and $\lambda_4 = \lambda_5$. In all other cases it is complex.

3. THE GROUP E_7

The algebra is of rank 7 and order 133. The Dynkin diagram is



The fundamental dominant weights are

$$\mathbf{\Pi}_1 = \begin{pmatrix}2&3&4&3&2&1\\&&2&&&\end{pmatrix}, \qquad \mathbf{\Pi}_2 = \tfrac{1}{2}\begin{pmatrix}2&4&6&5&4&3\\&&3&&&\end{pmatrix},$$

$$\mathbf{\Pi}_3 = \tfrac{1}{2}\begin{pmatrix}4&8&12&9&6&3\\&&7&&&\end{pmatrix}, \qquad \mathbf{\Pi}_4 = \begin{pmatrix}2&4&6&5&4&2\\&&3&&&\end{pmatrix},$$

$$\mathbf{\Pi}_5 = \begin{pmatrix}3&6&8&6&4&2\\&&4&&&\end{pmatrix}, \qquad \mathbf{\Pi}_6 = \tfrac{1}{2}\begin{pmatrix}6&12&18&15&10&5\\&&9&&&\end{pmatrix},$$

$$\mathbf{\Pi}_7 = \begin{pmatrix}4&8&12&9&6&3\\&&6&&&\end{pmatrix}. \tag{3.1}$$

The following seven roots are mutually orthogonal:

$$\mathbf{r}_1 = \begin{pmatrix}2&3&4&3&2&1\\&&2&&&\end{pmatrix}, \qquad \mathbf{r}_2 = \begin{pmatrix}0&1&2&2&2&1\\&&1&&&\end{pmatrix},$$

$$\mathbf{r}_3 = \begin{pmatrix}0&1&2&1&0&0\\&&1&&&\end{pmatrix}, \qquad \mathbf{r}_4 = \begin{pmatrix}0&1&0&0&0&0\\&&0&&&\end{pmatrix},$$

$$\mathbf{r}_5 = \begin{pmatrix}0&0&0&0&0&0\\&&1&&&\end{pmatrix}, \qquad \mathbf{r}_6 = \begin{pmatrix}0&0&0&1&0&0\\&&0&&&\end{pmatrix},$$

$$\mathbf{r}_7 = \begin{pmatrix}0&0&0&0&0&1\\&&0&&&\end{pmatrix}. \tag{3.2}$$

Hence all IUR's of E_7 are real.

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[1] M. L. Mehta, J. Math. Phys. 7, 1824 (1966). All the relevant references are given in that article.

The IUR's g_1, g_4, and g_5 have odd dimension numbers (cf. Appendix) and hence they are positive. The IUR's g_3 and g_6 are contained in $g_2 \times g_2 \times g_2$ and hence have the same sign[1] as g_2. The g_7 is contained in $g_1 \times g_1 \times g_1$ and hence is positive.

Now we show by an explicit construction that g_2 is negative.

The 56-dimensional IUR g_2 of the algebra E_7 is given by

$$H_i = -x_i p_i + y_i q_i + \sum x_{i\rho} p_{i\rho} - \sum y_{i\rho} q_{i\rho} - \tfrac{1}{3} \sum x_{\lambda\mu} p_{\lambda\mu} + \tfrac{1}{3} \sum y_{\lambda\mu} q_{\lambda\mu},$$

$$E_{(i)} = -\sum x_{\lambda} q_{i\lambda} - \sum x_{i\lambda} q_{\lambda},$$

$$E_{(ij)} = -x_i p_j + y_i q_j + \sum x_{i\rho} p_{j\rho} - \sum y_{j\rho} q_{i\rho},$$

$$E_{(ijk)} = -x_{ij} p_k - x_{jk} p_i - x_{ki} p_j + y_i q_{jk} + y_j q_{ki} + y_k q_{ij} - \sum y_{\lambda\mu} p_{\nu\rho},$$

$$E_{-(i)} = E^{+}_{(i)}, \qquad E_{-(ij)} = E^{+}_{(ij)}, \qquad E_{-(ijk)} = E^{+}_{(ijk)}, \tag{3.3}$$

$$x_{ik} = -x_{ki}, \qquad y_{ik} = -y_{ki},$$

$$p_i = \partial/\partial x_i, \qquad q_i = \partial/\partial y_i, \tag{3.4}$$

$$p_{ij} = \partial/\partial x_{ij}, \qquad q_{ij} = \partial/\partial y_{ij}, \qquad 1 \le i < j \le 7.$$

with the understanding that the various indices denoted by distinct indices are distinct, and in the expression of $E_{(ijk)}$, $ijk\lambda\mu\nu\rho$ forms an even permutation of the indices 1234567. Let us define C by

$$C = \sum_{i=1}^{7} (x_i q_i - y_i p_i) + \sum_{1 \le i < j \le 7} (x_{ij} q_{ij} - y_{ij} p_{ij}). \tag{3.5}$$

This matrix C transforms g_2 into g_2^*

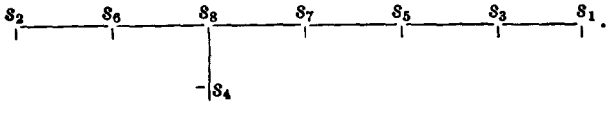
$$CLC^{-1} = -L^T, \tag{3.6}$$

where L is any of the matrices (3.3). The C in Eq. (3.5) above is clearly antisymmetric, showing that g_2 is real negative. We have thus proved the following theorem.

Theorem 8: All IUR's of E_7 are real. The sign of the IUR having the highest-weight $\sum \lambda_i \mathbf{\Pi}_i$ is given by $(-1)^{\lambda_2+\lambda_4+\lambda_6}$.

4. THE GROUP E_8

The algebra is of rank 8 and order 248. The Dynkin diagram is



The fundamental dominant weights are

$$\mathbf{\Pi}_1 = \begin{pmatrix} 2 & 4 & 6 & 5 & 4 & 3 & 2 \\ & & 3 & & & & \end{pmatrix}$$

$$\equiv 2\mathbf{s}_2 + 4\mathbf{s}_6 + 6\mathbf{s}_8 + 5\mathbf{s}_7 + 4\mathbf{s}_5 + 3\mathbf{s}_3 + 2\mathbf{s}_1 + 3\mathbf{s}_4,$$

$$\mathbf{\Pi}_2 = \begin{pmatrix} 4 & 7 & 10 & 8 & 6 & 4 & 2 \\ & & 5 & & & & \end{pmatrix},$$

$$\mathbf{\Pi}_3 = \begin{pmatrix} 4 & 8 & 12 & 10 & 8 & 6 & 3 \\ & & 6 & & & & \end{pmatrix}, \qquad \mathbf{\Pi}_4 = \begin{pmatrix} 5 & 10 & 15 & 12 & 9 & 6 & 3 \\ & & 8 & & & & \end{pmatrix},$$

$$\mathbf{\Pi}_5 = \begin{pmatrix} 6 & 12 & 18 & 15 & 12 & 8 & 4 \\ & & 9 & & & & \end{pmatrix}, \qquad \mathbf{\Pi}_6 = \begin{pmatrix} 7 & 14 & 20 & 16 & 12 & 8 & 4 \\ & & 10 & & & & \end{pmatrix},$$

$$\mathbf{\Pi}_7 = \begin{pmatrix} 8 & 16 & 24 & 20 & 15 & 10 & 5 \\ & & 12 & & & & \end{pmatrix}, \qquad \mathbf{\Pi}_8 = \begin{pmatrix} 10 & 20 & 30 & 24 & 18 & 12 & 6 \\ & & 15 & & & & \end{pmatrix}.$$

The following eight roots form an orthogonal system

$$\mathbf{r}_1 = \begin{pmatrix} 2 & 4 & 6 & 5 & 4 & 3 & 2 \\ & & 3 & & & & \end{pmatrix}, \qquad \mathbf{r}_2 = \begin{pmatrix} 2 & 3 & 4 & 3 & 2 & 1 & 0 \\ & & 2 & & & & \end{pmatrix},$$

$$\mathbf{r}_3 = \begin{pmatrix} 0 & 1 & 2 & 2 & 2 & 1 & 0 \\ & & 1 & & & & \end{pmatrix}, \qquad \mathbf{r}_4 = \begin{pmatrix} 0 & 1 & 2 & 1 & 0 & 0 & 0 \\ & & 1 & & & & \end{pmatrix},$$

$$\mathbf{r}_5 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ & & 0 & & & & \end{pmatrix}, \qquad \mathbf{r}_6 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & 1 & & & & \end{pmatrix},$$

$$\mathbf{r}_7 = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ & & 0 & & & & \end{pmatrix}, \qquad \mathbf{r}_8 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ & & 0 & & & & \end{pmatrix}.$$

The IUR g_1 is the regular representation. The IUR's g_2 and g_3 are contained in $g_1 \times g_1$, the g_4 and g_5 in $g_1 \times g_1 \times g_1$, the g_7 in $g_3 \times g_3$, the g_8 in $g_7 \times g_1$ and the g_6 in $g_2 \times g_2$. Thus

Theorem 9: All IUR's of E_8 are real positive.

ACKNOWLEDGMENT

We are thankful to Professor F. J. Dyson for suggesting this problem.

APPENDIX

The roots and fundamental dominant weights of the simple Lie algebras E_6, E_7, and E_8 with a possible choice of an orthonormal basis.

E_6

Roots:

$$\pm 2v_i, \qquad i = 1, 2, 3, 4;$$

$$\pm v_1 \pm v_2 \pm v_3 \pm v_4, \qquad \pm v_1 \pm v_2 \pm \sqrt{2}\, v_5, \qquad \pm v_3 \pm v_4 \pm \sqrt{2}\, v_5;$$

$$\pm v_1 \pm v_3 \pm \frac{1}{\sqrt{2}} (v_5 - \sqrt{3}\, v_6), \qquad \pm v_2 \pm v_4 \pm \frac{1}{\sqrt{2}} (v_5 - \sqrt{3}\, v_6);$$

$$\pm v_1 \pm v_4 \pm \frac{1}{\sqrt{2}} (v_5 + \sqrt{3}\, v_6), \qquad \pm v_2 \pm v_3 \pm \frac{1}{\sqrt{3}} (v_5 + \sqrt{3}\, v_6);$$

where v_i is a unit vector in the direction of the ith coordinate axis.

Simple roots:

$$2v_4, \qquad v_1 - v_2 - v_3 - v_4,$$

$$v_2 - v_3 \pm (1/\sqrt{2})(v_5 + \sqrt{3}\, v_6), \qquad v_3 - v_4 \pm \sqrt{2}\, v_5.$$

Fundamental dominant weights:

$$\Pi_1 = v_1 + v_2 + (\tfrac{2}{3})^{\frac{1}{2}} v_6, \qquad \Pi_2 = 2v_1,$$

$$\Pi_3 = v_1 + v_2 - (\tfrac{2}{3})^{\frac{1}{2}} v_6,$$

$$\Pi_4 = 2v_1 + v_2 + v_3 - (1/2^{\frac{1}{2}})v_5 + (1/6^{\frac{1}{2}})v_6,$$

$$\Pi_5 = 2v_1 + v_2 + v_3 + (1/2^{\frac{1}{2}})v_5 - (1/6^{\frac{1}{2}})v_6,$$

$$\Pi_6 = 3v_1 + v_2 + v_3 + v_4.$$

Dimensions of the fundamental representations:

27, 78, 27, 351, 351, 2925.

Order of the Weyl group: 72.6! = 51840.

E_7

Roots:

$$\pm v_1 \pm v_2 \pm v_3 \pm v_4, \qquad \pm v_1 \pm v_2 \pm v_5 \pm v_6,$$

$$\pm v_1 \pm v_3 \pm v_5 \pm v_7, \qquad \pm v_1 \pm v_4 \pm v_6 \pm v_7,$$

$$\pm v_2 \pm v_3 \pm v_6 \pm v_7, \qquad \pm v_2 \pm v_4 \pm v_5 \pm v_7$$

$$\pm v_3 \pm v_4 \pm v_5 \pm v_6, \qquad \pm 2v_i, \qquad i = 1, 2, \cdots, 7.$$

Simple roots:

$$v_1 - v_2 - v_3 - v_4, \qquad v_2 - v_3 - v_6 - v_7,$$

$$v_3 - v_4 - v_5 - v_6, \qquad 2v_4, \qquad 2v_5, \qquad 2v_6, \qquad 2v_7.$$

Fundamental dominant weights:

$$\Pi_1 = 2v_1, \qquad \Pi_2 = v_1 + v_2 + v_7,$$

$$\Pi_3 = 2v_1 + v_2 + v_3 + v_5, \qquad \Pi_4 = 2v_1 + 2v_2,$$

$$\Pi_5 = 3v_1 + v_2 + v_3 + v_4,$$

$$\Pi_6 = 3v_1 + 2v_2 + v_3 + v_6,$$

$$\Pi_7 = 4v_1 + 2v_2 + 2v_3.$$

Dimensions of the fundamental representations:

133, 56, 912, 1539, 8645, 27664, 365750.

Order of the Weyl group: 8.9! = 2903040.

E_8

Roots:

$$\pm v_5 \pm v_6 \pm v_7 \pm v_8, \qquad \pm v_3 \pm v_4 \pm v_7 \pm v_8,$$

$$\pm v_2 \pm v_4 \pm v_6 \pm v_8, \qquad \pm v_2 \pm v_3 \pm v_5 \pm v_8,$$

$$\pm v_1 \pm v_4 \pm v_5 \pm v_8, \qquad \pm v_1 \pm v_3 \pm v_6 \pm v_8,$$

$$\pm v_1 \pm v_2 \pm v_7 \pm v_8, \qquad \pm 2v_8,$$

in addition to those already listed under E_7.

Simple roots:

$$v_1 - v_2 - v_3 - v_4, \qquad v_2 - v_3 - v_5 - v_8,$$

$$v_3 - v_4 - v_5 - v_6, \qquad v_5 - v_6 - v_7 - v_8,$$

$$2v_4, \qquad 2v_6, \qquad 2v_7, \qquad 2v_8.$$

Fundamental dominant weights:

$$\Pi_1 = 2v_1, \qquad \Pi_2 = 2v_1 + 2v_2,$$

$$\Pi_3 = 3v_1 + v_2 + v_3 + v_4,$$

$$\Pi_4 = 3v_1 + 2v_2 + v_3 + v_5 + v_7,$$

$$\Pi_5 = 4v_1 + 2v_2 + 2v_3,$$

$$\Pi_6 = 4v_1 + 3v_2 + v_3 + v_5 + v_8,$$

$$\Pi_7 = 5v_1 + 3v_2 + 2v_3 + v_5 + v_6,$$

$$\Pi_8 = 6v_1 + 4v_2 + 2v_3 + 2v_5.$$

Dimensions of the fundamental representations:

248, 3875, 30380, 147250, 2450240, 6696000,

146325270, 6899079264.

Order of the Weyl group: 192.10! = 696729600.

Three-Dimensional Formulation of Gravitational Null Fields. I

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The four-dimensional normal hyperbolic Riemannian space is represented as a direct product of a three-dimensional space and a timelike line. The null gravitational field is defined in a manner analogous to that of electromagnetic field. It is shown that in this way three types of gravitational null fields can be characterized. We call them gravitational null fields of types A, B, and C. We find, as necessary and sufficient conditions, that the gravitational field be null field of types A and B, respectively. It is also shown that these null fields admit null vectors in accordance with the properties of gravitational radiation fields.

1. INTRODUCTION

In general relativity, owing to the nonlinear character of the field equations, it is exceedingly difficult to obtain exact information of a general nature. Therefore, one has to depend largely on either approximations or analogies from electromagnetic field, where the concept of radiation is well understood. However, the study of gravitational radiation from the point of weak-field approximation has not lead to any definite conclusion about gravitational radiation.[1,2,3,4] The reason for this is that the approximation procedure is not generally covariant; instead, the results are made to depend on a set of nontensor conditions known as the "coordinate conditions," the physical significance of which is obscure. It seems that these conditions impose restrictions on the geometry of space–time (under consideration), these restrictions are seldom desirable for the exact information of a general nature.

Trautman[5] has used the model of null electromagnetic field to formulate the boundary conditions for the asymptotic behavior of gravitational radiation fields. However, this treatment is approximate in nature. Also, Pirani[6] has been able to characterize gravitational radiation fields in an invariant manner basing on the fact that, in case of null electromagnetic fields, the timelike eigenvector of the stress-energy tensor collapses to the null cone.[7]

In this paper, we propose to obtain another criterion to characterize the gravitational radiation fields. This may be outlined as follows. Our sensory organs do not permit us to observe a 4–dimensional manifold in our immediate neighborhood; instead, we visualize this space–time region by performing observations in our rest-space in a sequence of different times. Because of this, we feel that, in discussing the problems of general relativity, we should pass from 4–dimensional formulation of the theory to a 3–dimensional one. Such a procedure is not novel and it has been used by several authors.

The worldline of an observer may be represented by a timelike congruence of curves. Let the unit vector, tangent to the worldline of an observer, be represented by u^p. Then we have[8]

$$u^p u_p = -1. \tag{1.1}$$

The kinematical properties of the "observers" can be studied with the help of this vector. For example, if we assume that u^p is a constant vector, then its existence is a necessary and sufficient condition for a space to be the direct product of a timelike line and a 3–space.[9] Of course, when u^p is a constant vector field the space–time is no longer Riemannian but Minkowskian. In this case, if a tensor is decomposed into two parts, orthogonal and tangential to u^p, then the orthogonal part will be just the Euclidean components of this tensor. This procedure is exactly analogous to the electromagnetic case where the field tensor F_{ab} is partitioned into two

[1] A. E. Scheidegger, Rev. Mod. Phys. **25**, 451 (1953).
[2] J. N. Goldberg, Phys. Rev. **99**, 1873 (1955).
[3] A. E. Scheidegger, Phys. Rev. **99**, 1883 (1955).
[4] H. Bondi and co-workers, however, have been able to develop an approximation procedure known as the "multipole expansion method" which is free from the objections raised here. See H. Bondi, Nature **186**, 535 (1960). H. Bondi, M. G. J. Van der Berg, and A. W. K. Metzner, Proc. Roy. Soc. (London) **A269**, 21 (1962).
[5] A. Trautman, "Lectures on General Relativity" (mimeographed notes), The University of London, Kings College (1958).
[6] F. A. E. Pirani, Phys. Rev. **105**, 1089 (1957).
[7] J. L. Synge, *Relativity, the Special Theory* (North-Holland Publishing Company, Amsterdam, 1958), Chap. IX.
[8] Our operational space is the normal hyperbolic Riemannian manifold with signature $+++-$. The range of small Latin indices is from 1 to 4 and those of Greek indices is from 1 to 3. Latin indices are used as tensor indices, whereas Greek indices shall be used as labels. If an index is given a particular value, it will be understood to be a label and not a tensor index. Labels as well as tensor indices will follow summation convention.
[9] J. Ehlers and W. Kundt, *Gravitation—An Introduction to Current Research*, L. Witten, Ed. (John Wiley & Sons, Inc., New York, 1962), Chap. 2.

3-vectors $\mathbf{E}$ and $\mathbf{H}$ in the three space with t = const. The electromagnetic radiation field is then defined by the following conditions

$$\mathbf{E}^2 = \mathbf{H}^2, \tag{1.2a}$$

$$\mathbf{E}\cdot\mathbf{H} = 0. \tag{1.2b}$$

The significance of these conditions is that, for a null electromagnetic field, the two vectors are equal in magnitude and are inclined to each other at a particular angle.[10]

We propose to apply a similar formalism for the discussion of gravitational null fields. We consider the tensor R_{abcd} as the basic field quantities, the analog of the electromagnetic field tensor F_{ab}. With the help of the curvature tensor and u^p (which we shall assume to be a general vectorfield), we construct three symmetric and traceless tensors, the analogs of $\mathbf{E}$ and $\mathbf{H}$. Different assumptions regarding the eigenvalues and eigenvectors of these tensors will provide us with the criterion for characterizing different types of gravitational fields.

In Sec. 2, we obtain different algebraic relations among these tensors. We confine ourselves to the case of vacuum gravitational fields. Later on, we also extend this concept to nonempty gravatitational fields. In Sec. 3, the criterion for gravitational null fields is given. It is found that three types of gravitational null fields can be defined. Secs. 4 and 5 are devoted to the study of these gravitational fields. In Sec. 6, the weak gravitational field has been discussed, and it has been shown that such linearized fields satisfy our criterion of null fields.

2. ALGEBRAIC PRELIMINARIES

The empty space–time of general relativity is characterized by the condition

$$R_{ij} = 0, \tag{2.1}$$

where R_{ij} is the contracted curvature tensor. The curvature tensor satisfies the following conditions[11]:

$$R_{ij(kl)} = R_{(ij)kl} = R_{i[jkl]} = 0. \tag{2.2}$$

Let the dual of a second-rank skew-symmetric tensor T_{ij} be defined as

$${}^{\times}T_{ij} = \tfrac{1}{2}\epsilon_{ijkl}T^{kl},$$

so that, with the help of R_{ijkl}, we can form the following duals:

$${}^{\times}R_{ijkl} = \tfrac{1}{2}\epsilon_{ijmn}R^{mn}_{kl}, \tag{2.3a}$$

$$R^{\times}_{ijkl} = \tfrac{1}{2}\epsilon_{klmn}R^{mn}_{ij}. \tag{2.3b}$$

We call ${}^{\times}R$ and $R^{\times}$ (indices suppressed) respectively the left dual and the right dual of R. It may easily be seen that the two duals are equal when (and only when)

$$R_{ij} - \tfrac{1}{4}g_{ij}R = 0. \tag{2.4}$$

Further, let us define

$${}^{\times\times}R_{ijkl} = \tfrac{1}{4}\epsilon_{ijmn}\epsilon_{klpv}R^{mnpv}. \tag{2.5}$$

If (2.1) holds, then we have[12]

$$R_{ijkl} = -{}^{\times\times}R_{ijkl}. \tag{2.6}$$

Now, we form the following tensors

$$G_{ik} = R_{ijkl}u^iu^l, \tag{2.7}$$

$$H_{ik} = {}^{\times}R_{ijkl}u^iu^l, \tag{2.8}$$

$$K_{ik} = {}^{\times\times}R_{ijkl}u^iu^l. \tag{2.9}$$

All these tensors satisfy

$$G^k_k = H^k_k = K^k_k = 0, \tag{2.10}$$

$$G_{[ij]} = H_{[ij]} = K_{[ij]} = 0. \tag{2.11}$$

It must be emphasized here that Eq. (2.10) is not valid in general but holds only for a vacuum field, i.e., under the condition (2.1). Equation (2.11) states that the tensors G, H, and K are symmetric; this is a consequence of the symmetry properties (2.2) of the curvature tensor. In general, they have rank three and lie in the space orthogonal to u^p. In view of (2.6), we also have

$$G_{ij} + K_{ij} = 0. \tag{2.12}$$

The curvature tensor has twenty algebraically different components. These are all contained in the tensors (2.7)–(2.9). Thus, the components of Riemann tensor are divided into three groups. This procedure is analogous to that of electromagnetic field where the tensor F_{ij}, in the 3-space t = const, is partitioned into two 3-vectors $\mathbf{E}(=F_{i4})$ and $\mathbf{H}(={}^{\times}F_{i4})$. If u^p is a constant vector field, then this decomposition is of local significance, because here, the space–time may be taken to be Minkowskian.

The Riemann tensor can be expressed in terms of (2.7), (2.8), and (2.9) as

$$\begin{aligned}(R + i{}^{\times}R)_{ijkl} &= (g + i\epsilon)_{ijmn}(g + i\epsilon)_{klpv}u^mu^p(G + iH)^{nv} \\ &= -(g + i\epsilon)_{ijmn}(g + i\epsilon)_{klpv}u^mu^p(K - iH)^{nv}.\end{aligned} \tag{2.13}$$

[10] In covariant form, Eqs. (1.2a) and (1.2b) are expressed as

$$F_{ij}F^{ij} = \tfrac{1}{2}\epsilon^{ijkl}F_{ij}F_{kl} = 0,$$

where ϵ^{ijkl} is the alternating symbol.

[11] The round brackets have been used for symmetrization and square brackets for skew-symmetrization.

[12] P. Jordan, J. Ehlers, and W. Kundt, Akad. Wiss. Abrandl. Math. Nat. Kl. 2, 23 (1960).

We observe from these equations that R_{ijkl} is described with the help of G_{ij} and H_{ij}. However, R_{ijkl} cannot be expressed, in general, in terms of G_{ij}, H_{ij}, and K_{ij}, and (2.13) is valid only when (2.1) is satisfied. Thus, different assumptions regarding the relationship between G_{ij} and H_{ij} will give rise to different gravitational situations. In particular, we shall define in the next section gravitational radiation fields by assuming the equality of G_{ij} and H_{ij}.

3. GRAVITATIONAL NULL FIELDS

As mentioned earlier, our aim is to find out the conditions for the gravitational field to be a null field. To fix our ideas, the model employed is that of the electromagnetic field, which entails the equality of the two 3–vectors and their relative orientation. Since the gravitational field is much more general than the electromagnetic field, we obtain three symmetric traceless tensors (2.7)–(2.9). Now, the condition of the equality of the 3–vectors has to be replaced by an appropriate condition regarding the nature of these tensors. Therefore, we make the following assumptions:

(A). *In order that the gravitational field be a radiation field, the tensor G_{ij} must be equal to H_{ij}. By equality of the tensors we mean the equality of the absolute eigenvalues.* This is the simplest assumption we can make regarding the nature of G_{ij} and H_{ij}. The question of relative orientation of the eigendirections has also to be taken into consideration. We consider G_{ij}, etc. as 3×3 matrices so that they have three eigendirections. In the case of null electromagnetic field, we know that **E** and **H** are symmetrically situated in the direction of propagation. This gives us (B) below.

(B). *If the gravitational field is a radiation field, then one of the eigenvectors corresponding to each of G_{ij} and H_{ij} is directed in the same direction, and the other two are symmetrically inclined to each other, i.e., at 45° to each other.*

In view of assumptions (A) and (B), we have to deal with the following cases.

(i) All the three eigenvalues of G_{ij} or H_{ij} are nonvanishing, then from (A) we obtain

$$G_{ij}G^{ij} = H_{ij}H^{ij}, \tag{3.1}$$

$$G_{ik}G^k_jG^{ij} = H_{ik}H^k_jH^{ij}. \tag{3.2}$$

Obviously, in this case, the rank of G_{ij} is three.

(ii) One of the eigenvalues of G_{ij} or H_{ij} is zero. This gives Eq. (3.1) and

$$G_{ik}G^k_jG^{ij} = H_{ik}H^k_jH^{ij} = 0. \tag{3.3}$$

The rank of G_{ij} will be 2.

(iii) All the eigenvalues of G_{ij} are zero. It is easy to see that Eqs. (3.1) and (3.3) will again hold. Thus we see that, in general, three types of gravitational null fields are possible. We term these gravitational null fields of types A, B, and C, respectively. We shall consider these one at a time.

4. GRAVITATIONAL NULL FIELDS OF TYPE A

In this section, we investigate the properties of the gravitational null fields of type A. Since (3.1) and (3.2) are assumed and (2.13) is valid, the geometric information of the curvature tensor is contained in G_{ij} and H_{ij}. This means that the geometry of R_{ijkl} can be obtained from the properties of G_{ij} and H_{ij}. Now, in this case, a coordinate system can be defined,

$$G_{ij} = \begin{pmatrix} -2A & 0 & 0 \\ 0 & A+B & 0 \\ 0 & 0 & A-B \end{pmatrix}, \tag{4.1}$$

$$H_{ij} = \begin{pmatrix} -2A & 0 & 0 \\ 0 & A & B \\ 0 & B & A \end{pmatrix}. \tag{4.2}$$

It is easy to see that (4.1) and (4.2) satisfy (2.10), (3.1), (3.2), and the assumptions (A) and (B).

For further discussion, it is convenient to use the nonholonomic coordinate frame defined with the help of unit eigenvectors e_i of G_{ij} and u_i. The vectors e_i satisfy

$$e_i e^{\beta i} = \delta^\beta_\alpha, \tag{4.3a}$$

$$e_i u^i = 0, \tag{4.3b}$$

and

$$g_{ij} = e_i e_j - u_i u_j. \tag{4.4}$$

The nonholonomic components of a tensor T_{ij} are then defined as

$$T_{\alpha\beta} = e^i e^j T_{ij}. \tag{4.5}$$

Now we state and prove the following theorems.

Theorem (4.1): In the 4–space with signature $+++-$, the necessary and sufficient condition that a vacuum gravitational field be a null gravitational field of type A is

$$\begin{aligned}[R_{abzv} + 2A(P-Q)_{abpq,xyrs} e^q_1 e^s_1 u^p u^r] \\ \times [R^{zvij} - A(P-Q)^{xymn,ijkl} e_{An} e_{Ai} u_m u_k] \\ \times [R_{cdij} - A(P-Q)_{cdef,ijgh} e^f_B e^h_B u^e u^g] = 0,\end{aligned} \tag{4.6}$$

where P and Q are defined as

$$P_{abpq,xyrs} = (g_{abpq}g_{xyrs} - \epsilon_{abpq}\epsilon_{xyrs}),$$

$$Q_{abpq,xyrs} = (g_{abpq}g_{xyrs} + g_{xyrs}\epsilon_{abpq}),$$

and A and B etc., range over 2 and 3.

Proof: It has been remarked earlier that the matrices (4.1) and (4.2) satisfy the postulates (A) and (B). Hence (4.1) and (4.2) represent a situation in which the gravitational field is a null field. We therefore verify that (4.6) is satisfied in view of (4.1) and (4.2), and then state conversely that the vanishing of the left-hand side of (4.6) is the necessary and sufficient condition for the field to be a null field of type A. In order to do this, we contract the left-hand side of (4.6) by $u^a u^c$, and obtain an equation which, upon further contraction by $e^b_1 e^d_1$, gives

$$H_{11} = -2A, \qquad H_{1A} = 0, \tag{4.7a}$$

if, in view of (4.1), the following equations are assumed,

$$G_{11} = -2A, \qquad G_{1A} = 0.$$

Similarly, on contraction by $e^b_2 e^d_2$ and $e^b_3 e^d_3$, respectively, and taking (4.1) into consideration, one obtains

$$H_{22} = \tfrac{1}{2}(G_{22} + G_{33}) = H_{33}, \tag{4.7b}$$

$$H_{23} = \tfrac{1}{2}(G_{22} - G_{33}) = H_{32}, \tag{4.7c}$$

which agree with (4.2). Thus conversely, the theorem is proved. G_{ij} and H_{ij} are therefore expressible in the forms (4.1) and (4.2); this shows that the eigenvectors have the required relative orientation, and that the eigenvalues have the required magnitudes.

Now, we shall show that the gravitational field, satisfying (4.6), admits a null vector (geodesic ray). This is true if the gravitational field is a radiation field.[13]

Theorem (4.2): If the gravitational field is a null-field of type A, then it defines a pencil of null vectors given by

$$k_a = u_a \pm e_{a1}, \tag{4.8}$$

which satisfy the Sach's equation[13]

$$R_{ijk[l}k_{m]}k^j k^k = 0. \tag{4.9}$$

Proof: It has been shown by Debever[14] that at any point of space–time, where the Riemann tensor does not vanish, there are null directions whose multiplicity adds exactly up to four. This is known as Debever's theorem. This can be most easily proved in the spinor formalism, as was first shown by Penrose.[15] Let us define the null directions as

$$k_a = Ae_{a1} + Be_{a2} + Ce_{a3} + Du_a,$$

where A, B, C, and D are scalars whose values are to be determined.

Substituting this values of k_a in (4.9) and taking (2.13), (3.1), (3.2), (4.1), and (4.2) into consideration, we obtain a system of equations in A, B, etc. Solving these we find that

$$B = C = 0, \qquad A = \pm D.$$

Thus, we obtain

$$k_a = D(u_a \pm e_{a1}).$$

Now, since a null vector defines a direction and not a magnitude, we can take, without loss of generality, $D = 1$. This proves the theorem. In the next section we consider the gravitational null field of type B.

5. GRAVITATIONAL NULL FIELDS OF TYPE B

In this case, Eqs. (3.1) and (3.3) are satisfied, since one of the eigenvalues is zero. We shall now establish the following theorem.

Theorem (5.1): If we define a tensor Q_{ijkl} as

$$Q_{ijkl} = R_{ijmn}R^{mn}_{kl}, \tag{5.1}$$

then the necessary and sufficient condition that an empty gravitational field is a null field of type B is that

$$Q_{ijkl} = 0. \tag{5.2}$$

Proof: In order to establish this theorem, we proceed as previously. Contracting the right-hand side of (5.1) by $u^i u^k$ we obtain

$$G_{jm}G^m_l = H_{jm}H^m_l, \tag{5.3}$$

so that from (5.3) we obtain (3.1). Similarly, if (5.1) is contracted by u^i, we obtain

$$G_{ij}H^i_k + H_{ij}G^i_k = 0. \tag{5.4}$$

Thus, from (5.3) and (5.4), we obtain (3.3).

Now, since one of the eigenvalues is zero, we can always choose a coordinate system in which

$$G_{1\alpha} = 0. \tag{5.5}$$

[13] R. K. Sachs, Proc. Roy. Soc. (London) **A264**, 309 (1961).
[14] R. Debever, Bull. Soc. Math. Belgique **10**, Fasc. 2, 112 (1959).
[15] R. Penrose, Ann. Phys. (N. Y.) **10**, 171 (1960).

We may further assume, without loss of generality, that

$$G_{23} = 0. \tag{5.6}$$

Now, contracting (5.3) by $e^i_1 e^l_1$ and making use of (5.5) and (5.6), we obtain $H_{1\alpha}H^{\alpha}_{1} = 0$ to get

$$H_{1\alpha} = 0. \tag{5.7}$$

Again, contracting (5.4) by $e^i_2 e^k_2$ and $e^i_3 e^k_3$, respectively, we obtain

$$H_{22} = H_{33} = 0. \tag{5.8}$$

Hence, from (5.3) we obtain

$$G^2_{22} = H^2_{23}. \tag{5.9}$$

The above considerations allow us to express G_{ij} and H_{ij} in the following form

$$G_{ij} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & A' & 0 \\ 0 & 0 & -A' \end{pmatrix}, \tag{5.10a}$$

$$H_{ij} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & A' \\ 0 & A' & 0 \end{pmatrix}. \tag{5.10b}$$

The two 3-tensors thus satisfy postulations (A) and (B), and hence the statement of the theorem.

Theorem (5.2): If the gravitational field is a null field of type B, then it defines a null vector k_a given by

$$k_a = u_a - e_{a}. \tag{5.11}$$
$$\quad\ 1$$

The vector k_a satisfies the equation

$$R_{ijkl}k^l = 0. \tag{5.12}$$

Proof: This theorem may be easily established if we proceed as in Theorem (4.2). The present theorem also states that all four Debever vectors in this case are coincident. In the next section, we will illustrate the linearized gravitational field as a field of gravitational radiation satisfying our definition of null fields.

6. EXAMPLES: WEAK GRAVITATIONAL FIELDS

In case of weak gravitational fields, the metric tensor can be expressed as the sum of Minkowskian metric η_{ij} and the deviation metric h_{ij}

$$g_{ij} = \eta_{ij} + h_{ij}, \tag{6.1}$$

where $\eta_{ij} = \text{diag. } (1, 1, 1, -1)$ and h_{ij} are small quantities of first order. The tensors G_{ij} and H_{ij} may be expressed in terms of h_{ij} as follows:

$$G_{ij} = \tfrac{1}{2}(h_{im,jk} + h_{jk,mi} - h_{ij,mk} - h_{km,ij})u^k u^m, \tag{6.2}$$

$$H_{ij} = \tfrac{1}{4}\epsilon_{ikpq}(h^{pm,q}_{\ \ j} + h^{q,pm}_{\ \ i} - h^{p,qm}_{\ \ i} - h^{qm,p}_{\ \ i})u^k u_m. \tag{6.3}$$

In order to investigate the contents of (6.2) and (6.3), let us introduce three spacelike constant unit vectors v_{α} orthogonal to each other and to u_i. We further define the quantities γ_{ij} as

$$\gamma_{ij} = h_{ij} - \tfrac{1}{2}\eta_{ij}\eta^{kl}h_{kl}, \tag{6.4}$$

and assume that the plane gravitational waves are functions of only v^i_1 and u^i directions. Then we obtain, as shown by Bergmann,[16]

$$G_{\alpha\beta} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \tfrac{1}{2}\gamma''_{33} & -\tfrac{1}{2}\gamma''_{23} \\ 0 & -\tfrac{1}{2}\gamma''_{23} & \tfrac{1}{2}\gamma''_{22} \end{pmatrix} \tag{6.5}$$

with[17]

$$\gamma_{22} + \gamma_{33} = 0. \tag{6.6}$$

Here a vector index has been replaced by a label as

$$A_{\alpha} = v^i_{\alpha} A_i. \tag{6.7}$$

In a similar manner, we also obtain

$$H_{\alpha\beta} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \tfrac{1}{2}\gamma''_{23} & \tfrac{1}{2}\gamma''_{33} \\ 0 & -\tfrac{1}{2}\gamma''_{22} & -\tfrac{1}{2}\gamma''_{23} \end{pmatrix}. \tag{6.8}$$

Equations (6.5) and (6.8) show that the eigenvalues are equal and the two tensors can be transformed into each other by a rotation of the 23 plane by an angle of $\frac{1}{4}\Pi$. Thus the linearized gravitational waves are gravitational null fields of type B.

Gravitational null fields of type C will be treated in another paper together with nonempty gravitational fields.

ACKNOWLEDGMENT

The authors are grateful to Professor D. Sharma for his encouragement and kind interest in this work.

[16] P. G. Bergmann, *Introduction to the Theory of Relativity* (Asia Publishing House, Bombay, 1960), p. 187.

[17] Primes denote differentiation with respect to $(v^i_1 - u^i)$.

Bipolar Expansion of Screened Coulomb Potentials, Helmholtz' Solid Harmonics, and their Addition Theorems

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Helmholtz' solid harmonics (spherical Bessel functions × spherical surface harmonics) are generated from fundamental spherical waves through a ladder procedure using raising and lowering operators. The addition theorem for them and the bipolar expansion formula of a screened Coulomb potential are derived. A method for evaluating two-center integrals with a general potential is given in the last section. This is new and useful in practical calculations. A key function

$$J^m_{ln}(x) = \frac{1}{2}\int_{-1}^{1} d\mu\, e^{i\mu x} P^m_l(\mu) P^m_n(\mu),$$

which appears in all the essential results, is studied in detail.

1. INTRODUCTION

In an essay[1] to explain the cohesive energy of He^4 at absolute-zero temperature, the author faced the need to expand a screened Coulomb potential $\exp(-\alpha\overline{PP'})/\overline{PP'}$ around two centers O and O' and utilized an expansion formula (1.1). As α tends to zero, it degenerates into the bipolar expansion of Coulomb potential obtained by Carlson and Rushbrooke.[2] One may find the formula (1.1) to have wider applications, e.g., in the calculation of the intermolecular binding energy. Buehler and Hirschfelder[3] supplemented Carlson and Rushbrooke's formula in the case of overlapping charge distributions, but their results are too complicated for practical use.

In quantum mechanics, on the other hand, especially in the problems of scattering and the structure of molecules, one often has to deal with partial spherical waves of the type

(spherical Bessel functions)

× (spherical surface harmonics),

which may appropriately be named *Helmholtz' solid harmonics*, because they are normal solutions of Helmholtz' wave equation

$$(\Delta + \alpha^2) f(\mathbf{r}) = 0.$$

Partial wave amplitudes of a general scattering process can be continued analytically into the complex l (angular momenta) plane, and their poles, "Regge poles," determine the high-energy behavior of related processes and provide a connection of this behavior with the bound states and resonances of the original process. Concerning recent studies in this field, the reader may be referred to Squires.[4]

The present paper gives the differential operators generating Helmholtz' solid harmonics from the fundamental (stationary and outgoing) spherical waves (in Sec. 3), the addition theorems for them (in Sec. 4), the bipolar expansion of an outgoing spherical wave (in Sec. 5), which is mathematically equivalent to the bipolar expansion of a screened Coulomb or Yukawa potential (1.1). The formulas are checked by using a method of divergent integrals and generalized functions in Sec. 7, and, in Sec. 8 a new method for evaluating two-center integrals with a general potential is given in a useful manner in practical calculations. The essential parts of the paper, except for Secs. 7 and 8, have been published in Japanese[5] and a part of them has been generalized by Tanabe.[6]

Let us take a common polar axis connecting the given centers O and O' with distance d apart and assume that a point P has the polar coordinates $(r, \cos^{-1}\mu, \varphi)$ with respect to the origin O and another point P' has $(r', \cos^{-1}\mu', \varphi')$ relative to the origin O'. See Fig. 1.

Then, the screened Coulomb potential is expanded

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[1] R. Nozawa and B. Sha, International Conference on Theoretical Physics, Abstracts for Symposium on Liquid Helium (Tokyo, 1953), p. 5.

[2] B. C. Carlson and G. S. Rushbrooke, Proc. Cambridge Phil. Soc. **46**, 626 (1950).

[3] R. J. Buehler and J. O. Hirschfelder, Phys. Rev. **83**, 628 (1951); **85**, 149 (1952).

[4] E. J. Squires, *Complex Angular Momenta and Particle Physics* (W. A. Benjamin, Inc., New York, 1963).

[5] R. Nozawa, Japan. J. Chem. & Solid State Phys. **35**, 75 (1954).

[6] Y. Tanabe, J. Phys. Soc. Japan **11**, 980 (1956).

around the two centers O and O′ in the following form:

$$\frac{\exp(-\alpha\overline{\mathrm{PP}'})}{\overline{\mathrm{PP}'}} = \alpha \sum_{l=0}^{\infty}\sum_{n=0}^{\infty}\sum_{m=0}^{[l,n]} (2l+1)(2n+1)P_l^m(\mu)P_n^m(\mu')\epsilon_m \cos m(\varphi-\varphi') \times (-)^l \begin{cases} i_l(\alpha r)i_n(\alpha r')K_{ln}^m(\alpha d), & r < \overline{\mathrm{OP}'},\ r' < d, \\ i_l(\alpha r)k_n(\alpha r')I_{ln}^m(\alpha d), & r < \overline{\mathrm{OP}'},\ r' > d, \\ k_l(\alpha r)i_n(\alpha r')I_{ln}^m(\alpha d), & r > \overline{\mathrm{OP}'}, \end{cases} \tag{1.1}$$

where $[l, n]$ denotes the lesser of l and n, ϵ_m is Neumann's factor, viz., $\epsilon_0 = 1$, $\epsilon_m = 2$ for $m \neq 0$, i_l and k_l are modified spherical Bessel functions defined by

$$i_l(x) = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} I_{l+\frac{1}{2}}(x),$$

$$k_l(x) = (-)^l\left(\frac{2}{\pi x}\right)^{\frac{1}{2}} K_{l+\frac{1}{2}}(x)$$

and

$$\left.\begin{matrix} K_{ln}^m(x) \\ I_{ln}^m(x) \end{matrix}\right\} = \sum_{h=m}^{[l,n]} \frac{(l-m)!\,(n-m)!\,(2h-1)!}{(l-h)!\,(n-h)!\,(h+m)!\,(h-m)!} \times \frac{1}{x^h}\begin{cases} k_{l+n-h}(x), \\ i_{l+n-h}(x). \end{cases} \tag{1.2}$$

The formula (1.1) is derived in Sec. 5 and (1.2) is proved in Sec. 6. When we make α vanish, formula (1.1) reduces to the bipolar expansion of Coulomb potential derived by Carlson and Rushbrooke[2]:

$$\frac{1}{\overline{\mathrm{PP}'}} = \sum_{l=0}^{\infty}\sum_{n=0}^{\infty}\sum_{m=0}^{[l,n]} P_l^m(\mu)P_n^m(\mu')\epsilon_m \cos m(\varphi-\varphi') \times \begin{cases} (-)^{n+m}\dfrac{(l+n)!}{(l+m)!\,(n+m)!}\dfrac{r^l r'^n}{d^{l+n+1}}, & r < \overline{\mathrm{OP}'},\ r' < d, \\ (-)^{l+n}\dfrac{(n-m)!}{(l+m)!\,(n-l)!}\dfrac{r^l d^{n-l}}{r'^{n+1}}, & r < \overline{\mathrm{OP}'},\ r' > d, \\ \dfrac{(l-m)!}{(n+m)!\,(l-n)!}\dfrac{r'^n d^{l-n}}{r^{l+1}}, & r > \overline{\mathrm{OP}'}, \end{cases} \tag{1.3}$$

which is rewritten in the form

$$\frac{1}{\overline{\mathrm{PP}'}} = \sum_{l=0}^{\infty}\sum_{n=0}^{\infty}\sum_{m=-[l,n]}^{[l,n]} P_l^m(\mu)P_n^{-m}(\mu')\exp[im(\varphi-\varphi')] \begin{cases} (-)^n\binom{l+n}{n-m}\dfrac{r^l r'^n}{d^{l+n+1}}, & r < \overline{\mathrm{OP}'},\ r' < d, \\ (-)^{l+n+m}\binom{n+m}{n-l}\dfrac{r^l d^{n-l}}{r'^{n+1}}, & r < \overline{\mathrm{OP}'},\ r' > d, \\ (-)^m\binom{l-m}{l-n}\dfrac{r'^n d^{l-n}}{r^{l+1}}, & r > \overline{\mathrm{OP}'}, \end{cases} \tag{1.4}$$

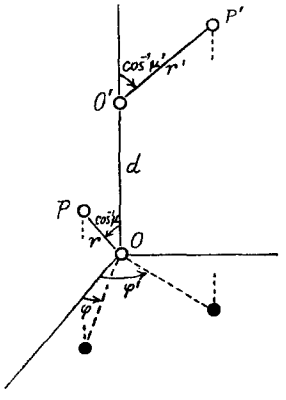

FIG. 1. The system of reference; O′ is the second center.

where $1/n!$ should be understood to vanish for negative integers n.

In order to derive (1.3) from (1.1), it is useful to replace the modified spherical Bessel functions $i_l(r)$ and $k_l(r)$ by their leading terms, cf. (2.12), and to pay attention to an identity

$$\sum_{m=h}^{[l,n]} (-)^h \frac{(2l+2n-2h-1)!!\,(2h-1)!!}{(l-h)!\,(n-h)!\,(h+m)!\,(h-m)!} = (-)^m \frac{(l+n)!\,(2l-1)!!\,(2n-1)!!}{(l-m)!\,(n-m)!\,(l+m)!\,(n+m)!}, \quad m \geq 0. \tag{1.5}$$

The validity of the identity (1.5) is verified by induction and is also known by comparing (6.5) with the first equality of (6.23).

2. DEFINITIONS AND BASIC FORMULAS

One occasionally encounters difficulties because several different definitions are used for Ferrers' functions. For $P_l^m(x)$, the Ferrers' function of order m associated with the Legendre polynomial of degree l, we adopt the definition

$$P_l^m(x) = \frac{(1-x^2)^{\frac{1}{2}m}}{2^l l!}\left(\frac{d}{dx}\right)^{l+m}(x^2-1)^l, \qquad -l \le m \le l. \tag{2.1}$$

Throughout the paper, l stands for a positive integer or zero, unless otherwise stated.

As usual, the mth derivative of Legendre polynomials is denoted by $P_l^{(m)}(x)$. An extension of this notation to negative m not less than $-l$ is often found useful. It is defined by

$$P_l^{(m)}(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^{l+m}(x^2-1)^l = \sum_{h=0}^{2h\le l-m}(-)^h\frac{(2l-2h-1)!!}{(l-m-2h)!\,(2h)!!}x^{l-m-2h}, \qquad -l \le m \le l. \tag{2.2}$$

Sometimes, it is convenient to understand $P_l^m(x)$ and $P_l^{(m)}(x)$ to vanish for $m > l$ by extending the definitions (2.1) and (2.2) and to vanish also for $m < -l$. The latter extension is consistent with (2.3) under the convention that $n! = 0$ for $n < 0$. Owing to the property that

$$P_l^{-m}(x) = (-)^m\frac{(l-m)!}{(l+m)!}P_l^m(x), \qquad -l \le m \le l, \tag{2.3}$$

orthogonality relations and the addition theorem for spherical surface harmonics are written in the forms

$$\int_{-1}^{1} d\mu\, P_l^m(\mu)P_n^{-m}(\mu) = (-)^m\frac{2}{2l+1}\delta_{ln}, \tag{2.4}$$

$$P_l(\mathbf{a}\vee\mathbf{b}) = \sum_{m=-l}^{l}(-)^m P_l^m(\mathbf{a}\vee\mathbf{c}) \times P_l^{-m}(\mathbf{b}\vee\mathbf{c})e^{im(\varphi_a-\varphi_b)}, \tag{2.5}$$

where $\mathbf{a}\vee\mathbf{b}$ means the cosine of the angle between the vectors $\mathbf{a}$ and $\mathbf{b}$, and φ_a, φ_b are the azimuthal angles of $\mathbf{a}$, $\mathbf{b}$ about $\mathbf{c}$ as the polar axis.

An intimate connection is conceived between Legendre polynomials and spherical Bessel functions by a glance at their recurrence relations:

$$\begin{cases}(2l+1)\mu P_l(\mu) = (l+1)P_{l+1}(\mu) + lP_{l-1}(\mu),\\ (2l+1)(d/dx)j_l(x) = lj_{l-1}(x) - (l+1)j_{l+1}(x),\end{cases}$$

$$\begin{cases}(2l+1)P_l(\mu) = (d/d\mu)P_{l+1}(\mu) - (d/d\mu)P_{l-1}(\mu),\\ [(2l+1)/x]j_l(x) = j_{l-1}(x) + j_{l+1}(x).\end{cases}$$

In fact, Legendre polynomials are connected with spherical Bessel functions by Fourier transforms:

$$\int_{-1}^{1} d\mu\, e^{ix\mu}P_l(\mu) = 2i^l j_l(x), \tag{2.6}$$

$$\int_{-\infty}^{\infty} dx\, e^{i\mu x}j_l(x) = \begin{cases}\pi i^l P_l(\mu), & |\mu| \le 1,\\ 0, & |\mu| > 1,\end{cases} \tag{2.7}$$

$$e^{i\mu x} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(x)P_l(\mu), \qquad |\mu| \le 1. \tag{2.8}$$

Here, the spherical Bessel, Neumann, and Hankel functions, $j_l(x)$, $n_l(x)$, and $h_l(x)$ are defined as follows:

$$\left.\begin{matrix}j_l(x)\\ n_l(x)\\ h_l(x)\end{matrix}\right\} = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}}\begin{cases}J_{l+\frac{1}{2}}(x)\\ Y_{l+\frac{1}{2}}(x) = (-)^{l+1}\left(\frac{\pi}{2x}\right)^{\frac{1}{2}}J_{-l-\frac{1}{2}}(x).\\ H^{(1)}_{l+\frac{1}{2}}(x)\end{cases} \tag{2.9}$$

Further, we define modified spherical Bessel functions, $i_l(x)$ and $k_l(x)$, by

$$\begin{aligned}i_l(x) &= (\pi/2x)^{\frac{1}{2}}I_{l+\frac{1}{2}}(x) = (-i)^l j_l(ix),\\ k_l(x) &= (-)^l(2/\pi x)^{\frac{1}{2}}K_{l+\frac{1}{2}}(x) = -(-i)^l h_l(ix).\end{aligned} \tag{2.10}$$

The spherical Hankel functions of the second kind, $h_l^{(2)}(x)$, are given on the real axis as the complex conjugate of $h_l(x)$,

$$h_l^{(2)}(x) = [h_l(x)]^* \quad \text{for real } x,$$

and are defined for complex z as their analytic continuation:

$$h_l(z) = j_l(z) + in_l(z), \quad h_l^{(2)}(z) = j_l(z) - in_l(z). \tag{2.11}$$

The leading terms for small argument are

$$\begin{cases}j_l(x) \to \dfrac{x^l}{(2l+1)!!},\\ n_l(x) \to (-)\dfrac{(2l-1)!!}{x^{l+1}},\end{cases}$$

$$\begin{cases}i_l(x) \to \dfrac{x^l}{(2l+1)!!},\\ k_l(x) \to (-)^l\dfrac{(2l-1)!!}{x^{l+1}},\end{cases} \tag{2.12}$$

$$\begin{cases}h_l(x) \to \dfrac{(2l-1)!!}{ix^{l+1}},\\ h_l^{(2)}(x) \to \dfrac{i(2l-1)!!}{x^{l+1}},\end{cases}$$

and the leading terms in the asymptotic expansions are

$$\begin{cases} j_l(x) \to \cos\,[x - \frac{1}{2}(l+1)\pi]/x, \\ n_l(x) \to \sin\,[x - \frac{1}{2}(l+1)\pi]/x, \\ i_l(x) \to e^x/2x, \\ k_l(x) \to (-)^l e^{-x}/x, \\ h_l(x) \to \exp\,(i[x - \frac{1}{2}(l+1)\pi])/x, \\ h_l^{(2)}(x) \to \exp\,(-i[x - \frac{1}{2}(l+1)\pi])/x. \end{cases} \tag{2.13}$$

Addition theorems for spherical waves read as follows: For the standing wave,

$$j_0(|\mathbf{r} - \mathbf{r}'|) = \sum_{l=0}^{\infty} (2l+1) j_l(r) j_l(r') P_l(\mathbf{r} \vee \mathbf{r}'). \tag{2.14}$$

For the outgoing wave,

$$h_0(|\mathbf{r} - \mathbf{r}'|) = \sum_{l=0}^{\infty} (2l+1) \begin{Bmatrix} j_l(r) h_l(r') \\ h_l(r) j_l(r') \end{Bmatrix} P_l(\mathbf{r} \vee \mathbf{r}'), \quad \begin{matrix} r < r', \\ r > r', \end{matrix}$$

where $\mathbf{r} \vee \mathbf{r}'$ means the cosine of the angle spanned by $\mathbf{r}$ and $\mathbf{r}'$.

We define Helmholtz' solid harmonics by

$$\begin{Bmatrix} J_l^m(\alpha\mathbf{r}) \\ H_l^m(\alpha\mathbf{r}) \end{Bmatrix} = i^l \begin{Bmatrix} j_l(\alpha r) \\ h_l(\alpha r) \end{Bmatrix} P_l^m(\mu) e^{im\varphi}, \qquad -l \le m \le l, \tag{2.15}$$

where $(r, \cos^{-1}\mu, \varphi)$ is the spherical coordinate of the point specified by the position vector $\mathbf{r}$. Evidently Helmholtz' solid harmonics $J_l^m(\mathbf{r})$ and $H_l^m(\mathbf{r})$ have the same parity as the spherical surface harmonics $Y_l^m(\cos^{-1}\mu, \varphi)$:

$$\begin{aligned} J_l^m(-\mathbf{r}) &= (-)^l J_l^m(\mathbf{r}), \\ H_l^m(-\mathbf{r}) &= (-)^l H_l^m(\mathbf{r}). \end{aligned} \tag{2.16}$$

Addition theorems, (2.14), for spherical waves are now written in the forms

$$j_0(|\mathbf{r} - \mathbf{r}'|) = \sum_{l=0}^{\infty} (-)^l (2l+1) \times \sum_{m=-l}^{l} (-)^m J_l^m(\mathbf{r}) J_l^{-m}(\mathbf{r}'), \tag{2.17}$$

$$h_0(|\mathbf{r} - \mathbf{r}'|) = \sum_{l=0}^{\infty} (-)^l (2l+1) \times \sum_{m=-l}^{l} (-)^m \begin{cases} J_l^m(\mathbf{r}) H_l^{-m}(\mathbf{r}'), & r < r', \\ H_l^m(\mathbf{r}) J_l^{-m}(\mathbf{r}'), & r > r', \end{cases}$$

and the expansion formula for the plane wave in terms of spherical waves is written as

$$e^{i\mathbf{k}\mathbf{r}} = \sum_{l=0}^{\infty} (2l+1) \sum_{m=-l}^{l} (-)^m J_l^m(k\mathbf{r}) P_l^{-m}(\mu_k) e^{-im\varphi_k}, \tag{2.18}$$

$(k, \cos^{-1}\mu_k, \varphi_k)$ being the polar expression for $\mathbf{k}$.

3. RAISING AND LOWERING OPERATORS

It is well known[7] that spherical solid harmonics of degree l are generated from $1/r$ by differential operators:

$$r^{-(l+1)} P_l^m(\cos\theta) e^{im\varphi} = (-)^l \frac{1}{(l-m)!} \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^m \left(\frac{\partial}{\partial z}\right)^{l-m} \frac{1}{r}, \qquad m \ge 0. \tag{3.1}$$

In view of the fact that a fundamental solution $e^{i\alpha r}/r$ of the Helmholtz equation $(\Delta + \alpha^2) f(\mathbf{r}) = 0$ goes to $1/r$ as α tends to zero, can we expect that Helmholtz' solid harmonics are derived from $h_0(\alpha r) = e^{i\alpha r}/i\alpha r$ by some differential operators?

An affirmative answer is furnished by the following formulas:

$$\begin{Bmatrix} H_l^m(\mathbf{r}) \\ J_l^m(\mathbf{r}) \end{Bmatrix} = (-i)^m \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^m P_l^{(m)}\left(-i\frac{\partial}{\partial z}\right) \begin{Bmatrix} h_0(r), \\ j_0(r), \end{Bmatrix} \tag{3.2}$$

$$\begin{Bmatrix} H_l^{-m}(\mathbf{r}) \\ J_l^{-m}(\mathbf{r}) \end{Bmatrix} = i^m \frac{(l-m)!}{(l+m)!} \left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)^m \times P_l^{(m)}\left(-i\frac{\partial}{\partial z}\right) \begin{Bmatrix} h_0(r), \\ j_0(r), \end{Bmatrix} \tag{3.3}$$

where $0 \le m \le l$ and $P_l^{(m)}(x)$ is the polynomial of degree $l - m$ defined by (2.2). It is verified that the formula (3.2) written for $H_l^m(\alpha\mathbf{r})$ multiplied by $-(-i\alpha)^{l+1}/(2l-1)!!$ degenerates into (3.1) as α tends to zero on account of the asymptotic relation (2.12).

In order to obtain the formulas (3.2) and (3.3), we develop a ladder procedure to utilize raising and lowering operators[8] for spherical Bessel functions and those for Ferrers' functions.

Let us define a differential operator $\mathfrak{R}_l$ by

$$\mathfrak{R}_l = (\partial/\partial r) - (l/r).$$

Then, $\mathfrak{R}_l$ is a raising, and $\mathfrak{R}_{-l-1}$ is a lowering,

[7] E. W. Hobson, *The Theory of Spherical and Ellipsoidal Harmonics* (Cambridge University Press, New York, 1931).

[8] E. Schrödinger, Proc. Roy. Irish Acad. **46**, 6 (1940); L. Infeld, Phys. Rev. **59**, 737 (1941); T. Inui, Progr. Theoret. Phys. (Kyoto) **3**, 168, 244 (1948); L. Infeld and T. E. Hull, Rev. Mod. Phys. **23**, 21 (1951).

operator for degree l of the spherical Bessel functions:

$$\mathfrak{R}_l\begin{Bmatrix} h_l(r) \\ j_l(r) \end{Bmatrix} = -\begin{Bmatrix} h_{l+1}(r) \\ j_{l+1}(r), \end{Bmatrix} \quad \mathfrak{R}_{-l-1}\begin{Bmatrix} h_l(r) \\ j_l(r) \end{Bmatrix} = \begin{Bmatrix} h_{l-1}(r) \\ j_{l-1}(r), \end{Bmatrix} \tag{3.4}$$

For Ferrers' functions $P_l^m(\cos\theta)$, it is useful to define a differential operator ϑ_l by

$$\vartheta_l = (\partial/\partial\theta) + (l+1)\cot\theta.$$

Then, the degree l is raised or lowered by unity by $\sin\theta\vartheta_l$ or $\sin\theta\vartheta_{-l-1}$, respectively, and the order m is raised or lowered by unity by ϑ_{-m-1} or ϑ_{m-1}, respectively:

$$\begin{aligned} &\sin\theta\cdot\vartheta_l P_l^m(\cos\theta) = (l-m+1)P_{l+1}^m(\cos\theta), \\ &\sin\theta\cdot\vartheta_{-l-1}P_l^m(\cos\theta) = -(l+m)P_{l-1}^m(\cos\theta). \\ &\vartheta_{-m-1}P_l^m(\cos\theta) = -P_l^{m+1}(\cos\theta), \\ &\vartheta_{m-1}P_l^m(\cos\theta) = (l+m)(l-m+1)P_l^{m-1}(\cos\theta). \end{aligned} \tag{3.5}$$

Once these formulas are known for nonnegative m, they are readily verified for negative m also, provided that $P_l^m(\cos\theta)$ are understood to vanish when $|m| > l$.

Now, since

$$\frac{\partial}{\partial x} + i\frac{\partial}{\partial y} = e^{i\varphi}\left(\sin\theta\frac{\partial}{\partial r} + \frac{\cos\theta}{r}\frac{\partial}{\partial\theta} + \frac{i}{r\sin\theta}\frac{\partial}{\partial\varphi}\right),$$

we have

$$\begin{aligned} &(2l+1)\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)H_l^m(\mathbf{r}) \\ &= (2l+1)\left(\sin\theta\frac{\partial}{\partial r} + \frac{\cos\theta}{r}\frac{\partial}{\partial\theta} - \frac{m}{r\sin\theta}\right)H_l^m(\mathbf{r})\cdot e^{i\varphi} \\ &= -\left[\left(\frac{\partial}{\partial r} - \frac{l}{r}\right)\left(\cos\theta\frac{\partial}{\partial\theta} - \frac{m}{\sin\theta} - (l+1)\sin\theta\right) + \left(\frac{\partial}{\partial r} + \frac{l+1}{r}\right)\left(-\cos\theta\frac{\partial}{\partial\theta} + \frac{m}{\sin\theta} - l\sin\theta\right)\right]H_l^m(\mathbf{r})e^{i\varphi} \\ &= -\left[\frac{1}{l-m}\mathfrak{R}_l\cdot\sin\theta\vartheta_l\cdot\vartheta_{-m-1} + \frac{1}{l+m+1}\mathfrak{R}_{-l-1}\cdot\sin\theta\vartheta_{-l-1}\cdot\vartheta_{-m-1}\right]H_l^m(\mathbf{r})e^{i\varphi} \\ &= i[H_{l+1}^{m+1}(\mathbf{r}) - H_{l-1}^{m+1}(\mathbf{r})], \end{aligned} \tag{3.6}$$

where use has been made of identities such as

$$\begin{aligned} \vartheta_l\vartheta_{-m-1}P_l^m(\cos\theta) &= [\vartheta_m + (l-m)\cot\theta]\vartheta_{-m-1}P_l^m(\cos\theta) \\ &= (l-m)[\cot\theta(\partial/\partial\theta) - m\operatorname{cosec}^2\theta - l - 1]P_l^m(\cos\theta). \end{aligned}$$

Although the above derivation has been done under the implicit assumption that $m \neq l$, the result is found to be valid still for $m = l$.

Similarly, we get

$$\begin{aligned} &(2l+1)\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)H_l^m(\mathbf{r}) \\ &= (2l+1)\left(\sin\theta\frac{\partial}{\partial r} + \frac{\cos\theta}{r}\frac{\partial}{\partial\theta} + \frac{m}{r\sin\theta}\right)H_l^m(\mathbf{r})\cdot e^{-i\varphi} \\ &= \left[\left(\frac{\partial}{\partial r} + \frac{l+1}{r}\right)\left(\cos\theta\frac{\partial}{\partial\theta} + \frac{m}{\sin\theta} + l\sin\theta\right) - \left(\frac{\partial}{\partial r} - \frac{l}{r}\right)\left(\cos\theta\frac{\partial}{\partial\theta} + \frac{m}{\sin\theta} - (l+1)\sin\theta\right)\right]H_l^m(\mathbf{r})e^{-i\varphi} \\ &= \left[-\frac{1}{l-m+1}\mathfrak{R}_{-l-1}\cdot\sin\theta\vartheta_{-l-1}\cdot\vartheta_{m-1} - \frac{1}{l+m}\mathfrak{R}_l\cdot\sin\theta\vartheta_l\cdot\vartheta_{m-1}\right]H_l^m(\mathbf{r})e^{-i\varphi} \\ &= i[(l+m)(l+m-1)H_{l-1}^{m-1}(\mathbf{r}) - (l-m+1)(l-m+2)H_{l+1}^{m-1}(\mathbf{r})], \end{aligned} \tag{3.7}$$

the result of which is verified for $m = -l$ also. While the differential operator

$$\frac{\partial}{\partial x} + i\frac{\partial}{\partial y} \quad \text{or} \quad \frac{\partial}{\partial x} - i\frac{\partial}{\partial y}$$

raises or lowers the order m of Helmholtz' solid harmonics, the operator $\partial/\partial z$ raises and lowers the degree l of them.

$$(2l+1)\frac{\partial}{\partial z}H_l^m(\mathbf{r})$$
$$= (2l+1)\left(\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}\right)H_l^m(\mathbf{r})$$
$$= [\mathfrak{R}_l\cdot\sin\theta\vartheta_l - \mathfrak{R}_{-l-1}\cdot\sin\theta\vartheta_{-l-1}]H_l^m(\mathbf{r})$$
$$= i[(l-m+1)H_{l+1}^m(\mathbf{r}) + (l+m)H_{l-1}^m(\mathbf{r})]. \quad (3.8)$$

The recurrence formulas (3.6) to (3.8) are valid even for negative m.

The formula (3.6) with both m and l replaced by $m-1$ reads:

$$H_m^m(\mathbf{r}) = -i(2m-1)\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)H_{m-1}^{m-1}(\mathbf{r}), \quad m \geq 0$$
$$= (-i)^m(2m-1)!!\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^m h_0(r), \quad (3.9)$$

and the formula (3.7) with m replaced by $-m+1$ and l replaced by $m-1$ becomes

$$H_m^{-m}(\mathbf{r}) = \frac{i}{2m}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)H_{m-1}^{-m+1}(\mathbf{r}), \quad m \geq 0$$
$$= \frac{i^m}{(2m)!!}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)^m h_0(r). \quad (3.10)$$

The formulas (3.2) and (3.3) result from (3.9) and (3.10) combined with the following relations:

$$H_l^m(\mathbf{r}) = \frac{1}{(2m-1)!!}P_l^{(m)}\left(-i\frac{\partial}{\partial z}\right)H_m^m(\mathbf{r}), \quad m \geq 0, \quad (3.11)$$

$$H_l^{-m}(\mathbf{r}) = (2m)!!\frac{(l-m)!}{(l+m)!}P_l^{(m)}\left(-i\frac{\partial}{\partial z}\right)H_m^{-m}(\mathbf{r}), \quad m \geq 0, \quad (3.12)$$

which may be proved by induction due to the recurrence formula (3.8).

The recurrence formulas (3.4) guarantee that the formulas (3.6) to (3.12) are valid also for $J_l^m(\mathbf{r})$ in place of $H_l^m(\mathbf{r})$.

4. ADDITION THEOREMS FOR HELMHOLTZ' SOLID HARMONICS

Here, we are concerned with the transformation of Helmholtz' solid harmonics under translation of the system of reference. Let a displacement of the origin be $\mathbf{d} = \overrightarrow{OO'}$ and choose it as the direction of the common polar axis, viz. z axis. Write $\mathbf{r}' =$

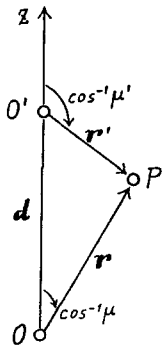

FIG. 2. The translation $\overrightarrow{OO'}$ of the system of reference.

$(r', \cos^{-1}\mu', \varphi')$ for the polar coordinates of P referred to the new origin O'. See Fig. 2.

Since the Helmholtz equation remains invariant under any translation of the Cartesian system of reference, Helmholtz' solid harmonics around O should be written in terms of those around O', and vice versa. Transformation formulas of such kind are called addition theorems.

The addition theorems for Helmholtz' solid harmonics are as follows:

$$\left.\begin{matrix}J_l^m(\mathbf{r})\\ H_l^m(\mathbf{r})\\ H_l^m(\mathbf{r})\end{matrix}\right\} = \frac{(l+m)!}{(l-m)!}\sum_{n=|m|}^{\infty}(2n+1)$$
$$\times\begin{cases}J_{ln}^{-m}(d)\,J_n^m(\mathbf{r}') \\ J_{ln}^{-m}(d)H_n^m(\mathbf{r}'), & d<r', \\ H_{ln}^{-m}(d)\,J_n^m(\mathbf{r}'), & d>r',\end{cases} \quad (4.1)$$

$$\left.\begin{matrix}J_l^m(\mathbf{r}')\\ H_l^m(\mathbf{r}')\\ H_l^m(\mathbf{r}')\end{matrix}\right\} = (-)^l\frac{(l+m)!}{(l-m)!}\sum_{n=|m|}^{\infty}(-)^n(2n+1)$$
$$\times\begin{cases}J_{ln}^{-m}(d)J_n^m(\mathbf{r}) \\ J_{ln}^{-m}(d)H_n^m(\mathbf{r}), & d<r, \\ H_{ln}^{-m}(d)J_n^m(\mathbf{r}) & d>r,\end{cases} \quad (4.2)$$

where m can be a negative integer and

$$J_{ln}^m(x) = \frac{1}{2}\int_{-1}^{1}d\mu\, e^{i\mu x}P_l^m(\mu)P_n^m(\mu)$$
$$= \sum_{k=|l-n|}^{l+n}i^k(2k+1)c_{kln}^m j_k(x), \quad (4.3)$$
$$H_{ln}^m(x) = \sum_{k=|l-n|}^{l+n}i^k(2k+1)c_{kln}^m h_k(x).$$

Here, the coefficient c_{kln}^m is given by

$$c_{kln}^m = \frac{1}{2}\int_{-1}^{1}d\mu\, P_k(\mu)P_l^m(\mu)P_n^m(\mu), \quad (4.4)$$

and hence it vanishes in either cases where $k > l + n$, $l > n + k$, $n > k + l$, $|m| > l$, or $|m| > n$.

The formulas (4.1) and (4.2), when written for $J_l^m(\alpha\mathbf{r})$ and $J_l^m(\alpha\mathbf{r}')$ both multiplied by $(2l + 1)!!$ $(i\alpha)^{-l}$ and for $H_l^m(\alpha\mathbf{r})$ and $H_l^m(\alpha\mathbf{r}')$ both multiplied by $-(-i\alpha)^{l+1}/(2l - 1)!!$, degenerate into addition theorems for spherical solid harmonics[7] as α tends to zero:

$$\begin{cases} r^l P_l^m(\mu) = \sum_{n=|m|}^{l} \binom{l+m}{l-n} d^{l-n} r'^n P_n^m(\mu'), \\ \dfrac{1}{r'^{l+1}} P_l^m(\mu) = \begin{cases} \sum_{n=l}^{\infty} (-)^{n-l} \binom{n-m}{n-l} \dfrac{d^{n-l}}{r'^{n+1}} P_n^m(\mu'), & d < r', \\ \sum_{n=|m|}^{\infty} (-)^{n+m} \binom{n+l}{n+m} \dfrac{r'^n}{d^{n+l+1}} P_n^m(\mu'), & d > r', \end{cases} \end{cases} \tag{4.5}$$

$$\begin{cases} r'^l P_l^m(\mu') = \sum_{n=|m|}^{l} (-)^{l-n} \binom{l+m}{l-n} d^{l-n} r^n P_n^m(\mu), \\ \dfrac{1}{r'^{l+1}} P_l^m(\mu') = \begin{cases} \sum_{n=l}^{\infty} \binom{n-m}{n-l} \dfrac{d^{n-l}}{r^{n+1}} P_n^m(\mu), & d < r, \\ (-)^{l-m} \sum_{n=|m|}^{\infty} \binom{n+l}{n+m} \dfrac{r^n}{d^{n+l+1}} P_n^m(\mu), & d > r, \end{cases} \end{cases} \tag{4.6}$$

where the factors $e^{im\varphi}$ and $e^{im\varphi'}$ are omitted on both sides for brevity.

In the process of derivation of (4.5) and (4.6) from (4.1) and (4.2), spherical Bessel and Hankel functions have been replaced by their leading terms, (2.12), and it is useful to notice that

$$c_{l-n\,l\,n}^m = \frac{(l+m)!\,(2n-1)!!\,(2l-2n-1)!!}{(2l+1)!!\,(l-n)!\,(n-m)!}, \quad l \geq n,$$

which is given in (6.21).

A straightforward proof of the formulas (4.1) for $m \geq 0$ is given by applying (3.2). Let us consider the addition theorems for spherical waves in the forms

$$\begin{Bmatrix} j_0(r) \\ h_0(r) \\ h_0(r) \end{Bmatrix} = \sum_{k=0}^{\infty} (2k+1) i^k \begin{Bmatrix} j_k(d) \\ j_k(d) \\ h_k(d) \end{Bmatrix} \times P_k\left(-i\frac{\partial}{\partial z'}\right) \begin{cases} j_0(r'), \\ h_0(r'), & d < r', \\ j_0(r'), & d > r'. \end{cases}$$

Apply to the both sides the differential operator

$$(-i)^m \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^m P_l^{(m)}\left(-i\frac{\partial}{\partial z}\right),$$

which is an invariant for translation of the reference system, and assume that the product of polynomials $P_l^{(m)}(x)$ and $P_k(x)$ is expanded in the form

$$P_k(x) P_l^{(m)}(x) = \sum_n (2n+1) \frac{(n-m)!}{(n+m)!} c_{kln}^m P_n^{(m)}(x), \tag{4.7}$$

which is known to be equivalent to (4.4) by multiplying both sides by $(1 - x^2)^{\frac{1}{2}m}$. The formulas (4.1), then, follow immediately.

Similarly, by applying (3.3), it is known that the formulas (4.1) are also valid for negative m. The formulas (4.2) are proved to be direct consequences of (4.1) by considering the inversion about the origin O and by recalling that Helmholtz' solid harmonics $J_l^m(\mathbf{r})$ and $H_l^m(\mathbf{r})$ have the parity of l.

5. BIPOLAR EXPANSION OF A SPHERICAL WAVE

The addition theorems for Helmholtz' solid harmonics facilitate the expansion of an outgoing spherical wave around two centers. Applying (2.17), we have

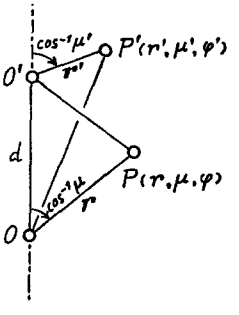

FIG. 3. The system of reference for double expansion.

$$h_0(\overline{PP'}) = \sum_{l=0}^{\infty} (-)^l(2l+1) \sum_{m=-l}^{l} (-)^m \begin{cases} H_l^m(\mathbf{r}) J_l^{-m}(\overrightarrow{OP'}), & r > \overline{OP'}, \\ J_l^m(\mathbf{r}) H_l^{-m}(\overrightarrow{OP'}), & r < \overline{OP'}, \end{cases}$$

of which $J_l^{-m}(\overrightarrow{OP'})$ and $H_l^{-m}(\overrightarrow{OP'})$ can be expanded in series of Helmholtz' solid harmonics around O' on account of (4.1). Thus we have

$$\begin{aligned} \frac{\exp(i\overline{PP'})}{i\overline{PP'}} &= \sum_{l=0}^{\infty} \sum_{n=0}^{\infty} (-)^l(2l+1)(2n+1) \frac{(l-m)!}{(l+m)!} \\ &\quad \times \sum_{m=-[l,n]}^{[l,n]} (-)^m \begin{cases} H_l^m(\mathbf{r}) J_n^{-m}(\mathbf{r}') J_{ln}^m(d), & r > \overline{OP'}, \\ J_l^m(\mathbf{r}) H_n^{-m}(\mathbf{r}') J_{ln}^m(d), & r < \overline{OP'}, \quad r' > d, \\ J_l^m(\mathbf{r}) J_n^{-m}(\mathbf{r}') H_{ln}^m(d), & r < \overline{OP'}, \quad r' < d, \end{cases} \\ &= \sum_{l=0}^{\infty} \sum_{n=0}^{\infty} i^{n-l}(2l+1)(2n+1) \sum_{m=0}^{[l,n]} \epsilon_m P_l^m(\mu) P_n^m(\mu') \cos[m(\varphi - \varphi')] \\ &\quad \times \begin{cases} h_l(r) j_n(r') J_{ln}^{-m}(d), & r > \overline{OP'}, \\ j_l(r) h_n(r') J_{ln}^{-m}(d), & r < \overline{OP'}, \quad r' > d, \\ j_l(r) j_n(r') H_{ln}^{-m}(d), & r < \overline{OP'}, \quad r' < d, \end{cases} \end{aligned} \tag{5.1}$$

where ϵ_m is Neumann's factor, $J_{ln}^m(x)$ and $H_{ln}^m(x)$ are the functions defined by (4.3) and can be expressed in the following forms, as shown in Sec. 6.1:

$$\left.\begin{matrix} J_{ln}^m(x) \\ H_{ln}^m(x) \end{matrix}\right\} = i^{l+n} \sum_{h=[m]}^{[l,n]} (-)^h \frac{(l+m)!\,(n+m)!\,(2h-1)!!}{(l-h)!\,(n-h)!\,(h+m)!\,(h-m)!} \frac{1}{x^h} \begin{cases} j_{l+n-h}(x), \\ h_{l+n-h}(x). \end{cases} \tag{5.2}$$

By replacing r, r', and d by ir, ir', and id, respectively, in (5.1) and (5.2), and by noticing that

$$\begin{aligned} J_{ln}^{-m}(ix) &= (-)^{l+n} I_{ln}^m(x), \\ H_{ln}^{-m}(ix) &= (-)^{l+n+1} K_{ln}^m(x), \end{aligned} \tag{5.3}$$

we attain the formula (1.1).

If we reverse the order of the procedure and expand the outgoing spherical wave first around O' according to the formula

$$h_0(\overline{PP'}) = \sum_{n=0}^{\infty} (-)^n(2n+1) \sum_{m=-n}^{n} (-)^m \begin{cases} H_n^{-m}(\mathbf{r}') J_n^m(\overrightarrow{O'P}), & r' > \overline{O'P}, \\ J_n^{-m}(\mathbf{r}') H_n^m(\overrightarrow{O'P}), & r' < \overline{O'P}, \end{cases}$$

then we have, by using (4.2),

$$\begin{aligned} \frac{\exp(i\overline{PP'})}{i\overline{PP'}} &= \sum_{l=0}^{\infty} \sum_{n=0}^{\infty} (-)^l(2l+1)(2n+1) \frac{(l-m)!}{(l+m)!} \\ &\quad \times \sum_{m=-[l,n]}^{[l,n]} (-)^m \begin{cases} J_l^m(\mathbf{r}) H_n^{-m}(\mathbf{r}') J_{ln}^m(d), & r' > \overline{O'P}, \\ H_l^m(\mathbf{r}) J_n^{-m}(\mathbf{r}') J_{ln}^m(d), & r' < \overline{O'P}, \quad r > d, \\ J_l^m(\mathbf{r}) J_n^{-m}(\mathbf{r}') H_{ln}^m(d), & r' < \overline{O'P}, \quad r < d, \end{cases} \end{aligned} \tag{5.4}$$

which can also be obtained directly from (5.1) by considering the inversion of the reference system.

6. THE FUNCTIONS $J_{ln}^m(\mathbf{x})$ AND $H_{ln}^m(\mathbf{x})$

In this section, the functions $J_{ln}^m(x)$ and $H_{ln}^m(x)$ are studied in detail, since they are key functions in the paper as seen from the formulas (4.1), (5.1), and (8.3), the last of which gives a new method for evaluating two-center integrals.

We have three methods for calculating $J^m_{ln}(x)$:

(1) Expansion formulas:

$$\left.\begin{matrix} J^m_{ln}(x) \\ H^m_{ln}(x) \end{matrix}\right\} = i^{l+n} \sum_{h=|m|}^{[l,n]} (-)^h \frac{(l+m)!\,(n+m)!\,(2h-1)!!}{(l-h)!\,(n-h)!\,(h+m)!\,(h-m)!} \frac{1}{x^h} \begin{cases} j_{l+n-h}(x), \\ h_{l+n-h}(x). \end{cases} \tag{6.1}$$

(2) Expansion formulas:

$$\left.\begin{matrix} J^m_{ln}(x) \\ H^m_{ln}(x) \end{matrix}\right\} = \sum_{k=|l-n|}^{l+n} i^k (2k+1) c^m_{kln} \begin{cases} j_k(x), \\ h_k(x). \end{cases} \tag{6.2}$$

The coefficient c^m_{kln} is given in forms of finite series:

$$c^m_{kln} = (-)^{g-l} \frac{g!\,k!\,(2g-2k)!\,(l+m)!}{(2g+1)!\,(g-k)!\,(g-l)!\,(g-n)!\,(l-m)!} \times \sum_t (-)^t \cdot \frac{(n+m+t)!}{(l-k+m+t)!\,t!} \cdot \frac{(l+k-m-t)!}{(n-m-t)!\,(k-t)!} \tag{6.3}$$

$$= (-)^g \frac{k!\,(l+m)!\,(n+m)!\,(2g-2k-1)!!\,(2g-2l-1)!!\,(2g-2n-1)!!}{(2g+1)!!} \times \sum_s \frac{(-)^s}{(s-l)!\,(s-n)!\,(s-k+m)!\,(l+n-m-s)!\,(k+l-s)!\,(k+n-s)!} \tag{6.4}$$

$$= (-)^{g-k} \frac{g!\,(l+m)!\,(n+m)!}{(2g+1)!\,(g-k)!} \sum_h \frac{(-)^h (2h)!\,(2g-2h)!}{(l-h)!\,(n-h)!\,(g-h)!\,(h+m)!\,(h-m)!\,(h-g+k)!}, \tag{6.5}$$

where $g = \frac{1}{2}(k+l+n)$ and c^m_{kln} vanishes when $k+l+n$ is odd. The summations in (6.3) to (6.5) are taken over all integral values of t, s, h for which the factorials are meaningful under the conventions:

$$1/n! = 0, \quad \text{for} \quad n < 0, \qquad 0! = 0!! = (-1)!! = 1.$$

(3) Recurrence formulas:

$$\begin{aligned} J^{m+1}_{ln}(x) &= (n-m)(n+m+1)J^m_{ln}(x) \\ &\quad - ix\left[\frac{(n+m)(n+m+1)}{2n+1} J^m_{l,n-1}(x) - \frac{(n-m)(n-m+1)}{2n+1} J^m_{l,n+1}(x)\right] \\ &= (l-m)(l+m+1)J^m_{ln}(x) \\ &\quad - ix\left[\frac{(l+m)(l+m+1)}{2l+1} J^m_{l-1,n}(x) - \frac{(l-m)(l-m+1)}{2l+1} J^m_{l+1,n}(x)\right], \end{aligned} \tag{6.6}$$

$$\frac{1}{2l+1}[(l-m+1)J^m_{l+1,n}(x) + (l+m)J^m_{l-1,n}(x)] = \frac{1}{2n+1}[(n-m+1)J^m_{l,n+1}(x) + (n+m)J^m_{l,n-1}(x)]. \tag{6.7}$$

The same formulas are also valid for $H^m_{ln}(x)$'s. The first subsection, 6.1, gives a method for deriving the formula (6.1). The formulas (6.3) to (6.5) are proved in Sec. 6.2, where some of recurrence relations for c^m_{kln} are given also. Following the subsection 6.3, where the recurrence formulas (6.6) and (6.7) are derived, an interesting property of the function $J^m_{ln}(x)$ is discussed in Sec. 6.4.

6.1. Derivation of the Formulas (6.1)

We make use of Gegenbauer's addition theorems[9] for spherical Bessel functions in the forms

$$\left.\begin{matrix} j_l(|\mathbf{r}-\mathbf{r}'|) \\ h_l(|\mathbf{r}-\mathbf{r}'|) \\ h_l(|\mathbf{r}-\mathbf{r}'|) \end{matrix}\right\} = \frac{|\mathbf{r}-\mathbf{r}'|^l}{(rr')^l} \sum_{h=l}^{\infty} (2h+1) \begin{Bmatrix} j_h(r)j_h(r') \\ j_h(r)h_h(r') \\ h_h(r)j_h(r') \end{Bmatrix} P^{(l)}_h(\mathbf{r} \vee \mathbf{r}'), \qquad \begin{matrix} r < r', \\ r > r', \end{matrix} \tag{6.8}$$

[9] G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, New York, 1944).

where $\mathbf{r} \vee \mathbf{r}'$ denotes the cosine of the angle spanned by $\mathbf{r}$ and $\mathbf{r}'$ both referred to the same origin, and $P_k^{(l)}(x)$ is defined by (2.2). A useful comment on it is that

$$P_k^{(l)}(-x) = (-)^{k-l}P_k^{(l)}(x).$$

We introduce here two sorts of integral operations; one is the spherical average around the center O after multiplication by $P_l^m(\mu)\exp(-im\varphi)$, cf. Fig. 3:

$$S_{lm}^0 \equiv (4\pi)^{-1}\int_{-1}^{1} d\mu \int_0^{2\pi} d\varphi\, P_l^m(\mu)\exp(-im\varphi)\times,$$

the other is the spherical average around the second center O′ after multiplication by $P_n^m(\mu')\exp(im\varphi')$:

$$S_{nm}^{0'} \equiv (4\pi)^{-1}\int_{-1}^{1} d\mu' \int_0^{2\pi} d\varphi'\, P_n^m(\mu')\exp(im\varphi')\times.$$

Then we get

$$S_{nm}^{0'}[h_0(\overline{\mathrm{PP}'})] = \begin{Bmatrix} j_n(r')h_n(\overline{\mathrm{O'P}}) \\ h_n(r')j_n(\overline{\mathrm{O'P}}) \end{Bmatrix} P_n^m(\overrightarrow{\mathrm{O'P}} \vee \overrightarrow{\mathrm{OO'}}) \times \exp(im\varphi), \qquad \begin{matrix} r' < \overline{\mathrm{O'P}}, \\ r' > \overline{\mathrm{O'P}}. \end{matrix}$$

After the spherical Bessel functions $h_n(\overline{\mathrm{O'P}})$ and $j_n(\overline{\mathrm{O'P}})$ are expanded by using Gegenbauer's addition theorems (6.8), the addition theorem for spherical solid harmonics, (4.6), can be applied to $\overline{\mathrm{O'P}}^n P_n^m(\overrightarrow{\mathrm{O'P}} \vee \overrightarrow{\mathrm{OO'}})$.

If we confine ourselves to the case where $r + r' < d$ for the moment, we get

$$S_{lm}^0[S_{nm}^{0'}h_0(\overline{\mathrm{PP}'})] = j_n(-r')JH_{ln}(r, d),$$

where

$$JH_{ln}(r, d) = \frac{1}{2r^n}\sum_{k=0}^{n}(-)^k\binom{n+m}{n-k}\left(\frac{r}{d}\right)^k \times \sum_{h=0}^{k+l-n}(2h+1)b_{mkl}^{nh}j_h(r)h_h(d), \tag{6.9}$$

$$b_{mkl}^{nh} = \int_{-1}^{1} d\mu\, P_h^{(n)}(\mu)P_k^m(\mu)P_l^m(\mu), \tag{6.10}$$

which is to be understood to vanish in either case where $h < n$, $k < |m|$, or $l < |n|$.

When the order of performance of the spherical averages are reversed, we have

$$S_{nm}^{0'}[S_{lm}^0 h_0(\overline{\mathrm{PP}'})] = j_l(r)JH_{nl}(-r', d),$$

where $JH_{nl}(-r', d)$ stands for an expression derived from $JH_{ln}(r, d)$, (6.9), by replacing r by $-r'$ after exchanging l and n. As the results of the spherical averages should coincide with each other, we obtain an identity

$$\frac{JH_{ln}(r, d)}{j_l(r)} = \frac{JH_{nl}(-r', d)}{j_n(-r')} \equiv F(d), \qquad r + r' < d.$$

The value of the identity has been denoted by $F(d)$, since it can depend neither on r nor on r'.

A simplified expression for $F(d)$ is obtained by making r tend to zero and by replacing spherical Bessel functions by their leading terms:

$$F(d) = \frac{(2l+1)!!}{2}\sum_{k=0}^{n}(-)^k\binom{n+m}{n-k} \times \frac{2l+2n-2k+1}{(2l+2n-2k+1)!!}\, b_{mkl}^{nl+n-k}\,\frac{h_{l+n-k}(d)}{d^k}.$$

The coefficient b_{mkl}^{nh}, (6.10), is integrated out for $h = l + n - k$:

$$\begin{aligned} b_{mkl}^{nl+n-k} &= (-)^m\frac{(l+m)!}{(l-m)!}\int_{-1}^{1} d\mu\, P_l^{(-m)}(\mu)P_k^{(m)}(\mu)P_{l+n-k}^{(n)}(\mu) \\ &= (-)^l\frac{(l+m)!}{(2l)!!\,(l-m)!}\int_{-1}^{1} d\mu\cdot(\mu^2-1)^l\left(\frac{d}{d\mu}\right)^{l-m}[P_k^{(m)}(\mu)P_{l+n-k}^{(n)}(\mu)] \\ &= \frac{(l+m)!\,(2k-1)!!\,(2l+2n-2k-1)!!}{(2l)!!\,(k-m)!\,(l-k)!}\int_{-1}^{1} d\mu\,(1-\mu^2)^l \\ &= \frac{2\cdot(l+m)!\,(2k-1)!!\,(2l+2n-2k-1)!!}{(2l+1)!!\,(k-m)!\,(l-k)!}, \quad \text{when} \quad |m| \le k \le l, \\ &= 0, \qquad \text{otherwise.} \end{aligned} \tag{6.11}$$

Thus we find a simplified expression:

$$F(d) = \sum_{k=|m|}^{[l,n]}(-)^k\frac{(l+m)!\,(n+m)!\,(2k-1)!!}{(l-k)!\,(n-k)!\,(k+m)!\,(k-m)!}\frac{1}{d^k}\,h_{l+n-k}(d). \tag{6.12}$$

If we use the bipolar expansion (5.1) for $h_0(\overline{PP'})$ in $S^0_{lm}[S^{0'}_{nm}h_0(\overline{PP'})]$, we obtain a relation

$$H^m_{ln}(d) = i^{l+n}F(d). \tag{6.13}$$

In the case where $r' + d < r$ or $r + d < r'$, the results of the successive spherical averages are given as follows:

$$S^0_{lm}[S^{0'}_{nm}h_0(\overline{PP'})] = \begin{cases} j_n(-r')HJ_{ln}(r, d), & r' + d < r, \\ (-)^n h_n(r')JJ_{ln}(r, d), & r + d < r', \end{cases}$$

$$S^{0'}_{nm}[S^0_{lm}h_0(\overline{PP'})] = \begin{cases} h_l(r)JJ_{nl}(r', -d), & r' + d < r, \\ j_l(r)HJ_{nl}(r', -d), & r + d < r'. \end{cases}$$

Here $HJ_{ln}(r, d)$ is an expression obtained from $JH_{ln}(r, d)$, (6.9), by exchanging two spherical Bessel functions j_h and h_h, and $JJ_{ln}(r, d)$ is that obtained from $JH_{ln}(r, d)$ by replacing h_h by j_h.

Again, comparison leads us to the identities

$$\frac{HJ_{ln}(r, d)}{h_l(r)} = \frac{JJ_{nl}(r', -d)}{j_n(-r')} \equiv G(d), \qquad r' + d < r,$$

$$\frac{JJ_{ln}(r, d)}{j_l(r)} = \frac{HJ_{nl}(r', -d)}{(-)^n h_n(r')} \equiv H(d), \qquad r + d < r'.$$

By letting $r' \to 0$ in $G(d)$, and $r \to 0$ in $H(d)$, it is known that $G(d)$ coincides with $H(d)$ and is given by

$$G(d) = H(d) = \sum_{k=|m|}^{[l,n]} (-)^k \times \frac{(l + m)!\,(n + m)!\,(2k - 1)!!}{(l - k)!\,(n - k)!\,(k + m)!\,(m - k)!}\,\frac{1}{d^k}\,j_{l+n-k}(d). \tag{6.14}$$

We can find also the relations

$$J^m_{ln}(x) = i^{l+n}G(d) = i^{l+n}H(d) \tag{6.15}$$

by substituting the bipolar expansion (5.1) for $h_0(\overline{PP'})$ in $S^0_{lm}[S^{0'}_{nm}h_0(\overline{PP'})]$. The formulas (6.1) are an immediate result of the combination of (6.13) with (6.12) and of (6.15) with (6.14).

6.2. Properties of the Coefficient c^m_{kln}

Next, we derive useful formulas for the coefficient c^m_{kln}:

$$c^m_{kln} = \frac{1}{2}\int_{-1}^{+1} d\mu\, P_k(\mu)P^m_l(\mu)P^m_n(\mu).$$

(6.3) is a special form of Gaunt's formula[10]

$$\int_{-1}^{1} d\mu\, P^s_k(\mu)P^w_l(\mu)P^{s+w}_n(\mu) = (-)^{g-l-s}\,\frac{2\cdot g!\,(k + v)!\,(l + w)!\,(l + n - k)!}{(2g + 1)!\,(g - k)!\,(g - l)!\,(g - n)!\,(l - w)!} \times \sum_t (-)^t \frac{(l + k - v - w - t)!\,(n + v + w + t)!}{(l - k + v + w + t)!\,(n - v - w - t)!\,(k - v - t)!\,t!}. \tag{6.16}$$

The integral vanishes except when the sum $k + l + n$ is even and k, l, n obey the triangular relation:

$$l + n \geq k \geq |l - n|, \quad l + k \geq n, \quad k + l + n = 2g.$$

In order to pass from (6.3) to (6.4) which has a symmetrical form with respect to l and n, the following identity is used most conveniently:

$$\frac{a!}{b!\,c!} = \sum_u \frac{(a-b)!\,(a-c)!}{(a-b-u)!\,(a-c-u)!\,(b+c-a+u)!\,u!} \qquad a \geq b, \quad a \geq c. \tag{6.17}$$

This is a special form of the addition theorem for binomial coefficients:

$$\sum_{s=\max(0,n-y)}^{\min(x,n)} \binom{x}{s}\binom{y}{n-s} = \binom{x+y}{n}, \tag{6.18}$$

where x, y, n are natural numbers such that $x + y \geq n$, or Vandermonde's theorem[11]

$$\sum_{s=0}^{n} \binom{n}{s} x(x-1)\cdots(x-s+1) \times y(y-1)\cdots(y-n+s+1) = (x + y)(x + y - 1)\cdots(x + y - n + 1), \tag{6.19}$$

which is valid for any complex numbers x and y with the understanding that

$$x(x-1)\cdots(x-s+1) = \Gamma(x+1)/\Gamma(x-s+1)$$

as long as n is an integer.

Applying (6.17) to each of the fractional factors

[10] J. A. Gaunt, Phil. Trans. Roy. Soc. (London) **A228**, 194 (1929).

[11] For example, G. Chrystal, *Text Book of Algebra II* (A. and C. Black, Ltd., London, 1900), 2nd ed., p. 9.

under the summation symbol in (6.3), we get

$$c^m_{kln} = (-)^{g-l}\frac{g!\,k!\,(2g-2k)!\,(2g-2l)!\,(2g-2n)!\,(l+m)!\,(n+m)!}{(2g+1)!\,(g-k)!\,(g-l)!\,(g-n)!}$$

$$\times \sum_{t,u,v}\frac{(-)^t}{(k+n-l-u)!\,(n+m-u)!\,(-k+l-n+t+u)!\,u!\,(k+l-n-v)!\,(l-m-v)!\,(n-l-t+v)!\,v!}.$$

The triple sum over t, u, v reduces to a single one

$$\sum_u (-)^{k-l+n-u}\frac{1}{(k+n-l-u)!\,(n+m-u)!\,u!\,(u+l-n)!\,(u+l-m-k)!\,(k-u)!}$$

on account of the identity

$$\sum_t \frac{(-)^t}{(t-a)!\,(b-t)!} = (-)^a\delta_{a,b}.$$

Thus, by replacing the running number u by $k+n-s$, we have (6.4).

Now we turn to the derivation of (6.5). Expand the function $x^{-k}j_{l+n-k}(x)$ in (6.1) into a series of $j_k(x)$'s by an identity

$$\frac{1}{x^k}j_l(x) = \sum_{k=l-h}^{l+h}\binom{h}{\frac{1}{2}(l+h-k)}$$

$$\times \frac{(k+l-h-1)!!\,(2k+1)}{(k+l+h+1)!!}\,j_k(x), \qquad h \le l, \tag{6.20}$$

where k runs in steps of two units. This is a generalized form of the first of the recurrence formulas (A1). Then, comparison of the result with (6.2) yields (6.5) immediately by virtue of the orthogonality of $j_l(x)$'s:

$$\int_{-\infty}^{\infty} dx\, j_l(x)j_n(x) = \frac{\pi}{2l+1}\,\delta_{ln},$$

which is shown in the Appendix, (A2).

The series (6.3)–(6.5) are known to be summed up only in few cases:

$$c^0_{kln} = \frac{(k+l+n)!!}{(k+l+n+1)!!}\,\frac{(k+l-n-1)!!}{(k+l-n)!!}\,\frac{(l+n-k-1)!!}{(l+n-k)!!}\,\frac{(n+k-l-1)!!}{(n+k-l)!!},$$

$$c^m_{l+n,l,n} = (-)^m\frac{(2l)!\,(2n)!\,(l+n)!\,(l+n)!}{l!\,n!\,(l-m)!\,(n-m)!\,(2l+2n+1)!},$$

$$c^m_{l-n,l,n} = \frac{(2l-2n)!\,(2n)!\,l!\,(l+m)!}{(l-n)!\,(l-n)!\,n!\,(2l+1)!\,(n-m)!}, \qquad l \ge n, \tag{6.21}$$

$$c^n_{kln} = (-)^{\frac{1}{2}(k-l+n)}\frac{(l+n)!\,(2n)!\,(k+l-n-1)!!}{(l-n)!\,(k+l+n+1)!!\,(l-k+n)!!\,(k+n-l)!!},$$

$$c^g_{kln} = (-)^k\frac{g!\,(l+g)!\,(n+g)!}{(2g+1)!\,k!\,(g-k)!\,(l-g)!\,(n-g)!}, \qquad l,n \ge g,$$

$$c^m_{0ln} = \delta_{l,n}\frac{1}{2l+1}\frac{(l+m)!}{(l-m)!}.$$

The first is given in Hobson's monograph[7] and is tabulated for $g \le 4$ in Table I in the Appendix. The second is obtained by taking $k = l+n$ in (6.3), the third and the fourth result from (6.4) by putting $k = l-n$ and $m = n < l$, respectively. The second expression is obtained also from (6.5) by comparing it with the identity (1.5). The fourth and the fifth come from (6.5), and the last is a trivial case where all the series in (6.3) to (6.5) degenerate into a single term.

Other special values of the coefficient c^m_{kln} are obtained by expanding the product $P^m_l(\mu)P^m_n(\mu)$ in a polynomial with descending powers of μ, which is obtained by (2.2). The first three terms are

$$(-)^m(l-m)!\,(n-m)!\,P_l^m(\mu)P_n^m(\mu) = (2l-1)!!\,(2n-1)!!\,\mu^{l+n} - \frac{1}{2!!}(2l-3)!!\,(2n-3)!!\,(l+n-1)$$

$$\times [(2ln - l - n) + 2m^2]\mu^{l+n-2} + \frac{4}{4!!}(2l-5)!!\,(2n-5)!!\,(l+n-2)(l+n-3)$$

$$\times [ln(ln - 2l - 2n + 2) + (2ln - 3l - 3n + 2)m^2 + m^4]\mu^{l+n-4} + \cdots \tag{6.22}$$

from which we have

$$c^m_{l+n,l,n} = (-)^m \frac{(2l-1)!!\,(2n-1)!!\,(l+n)!}{(l-m)!\,(n-m)!\,(2l+2n+1)!!},$$

$$c^m_{l+n-2,l,n} = (-)^m \frac{(2l-3)!!\,(2n-3)!!\,(l+n-1)!}{(l-m)!\,(n-m)!\,(2l+2n-1)!!}[ln - (2l+2n-1)m^2], \tag{6.23}$$

$$c^m_{l+n-4,l,n} = (-)^m \frac{(2l-5)!!\,(2n-5)!!\,(l+n-2)!}{2!!\,(l-m)!\,(n-m)!\,(2l+2n-3)!!}$$

$$\times [3ln(l-1)(n-1) + (2l+2n-3)(6ln + 4l + 4n - 1)m^2 + (2l+2n-3)(2l+2n-5)m^4],$$

on account of the formula

$$\int_{-1}^{1} d\mu\, P_k(\mu)\mu^n = \begin{cases} \dfrac{2\cdot n!}{(n-k)!}\dfrac{(n-k-1)!!}{(n+k+1)!!}, & \text{for } n \geq k, \\ 0, & \text{for } k > n. \end{cases} \tag{6.24}$$

The first of (6.23) coincides with the second of (6.21).

Some recurrence relations for c^m_{kln} are listed below:

$$\frac{k+1}{2k+1}c^m_{k+1,l,n} + \frac{k}{2k+1}c^m_{k-1,l,n} = \frac{l-m+1}{2l+1}c^m_{k,l+1,n} + \frac{l+m}{2l+1}c^m_{k,l-1,n}$$
$$= \frac{n-m+1}{2n+1}c^m_{k,l,n+1} + \frac{n+m}{2n+1}c^m_{k,l,n-1}, \tag{6.25}$$

$$(l+n-k)(l+n-k+2)c^m_{k-2,l,n} = (k+l+n-1)(k+l+n+1)c^m_{kln}$$
$$- \frac{2k-1}{l-n}[(2l-1)(l+m)c^m_{k-1,l-1,n} - (2n-1)(n+m)c^m_{k-1,l,n-1}], \tag{6.26}$$

$$\begin{cases} \dfrac{1}{2l+1}(c^{m+1}_{k,l+1,n} - c^{m+1}_{k,l-1,n}) = \dfrac{(n+m)(n+m+1)}{2n+1}c^m_{k,l,n-1} - \dfrac{(n-m)(n-m+1)}{2n+1}c^m_{k,l,n+1}, \\ \dfrac{1}{2n+1}(c^{m+1}_{k,l,n+1} - c^{m+1}_{k,l,n-1}) = \dfrac{(l+m)(l+m+1)}{2l+1}c^m_{k,l-1,n} - \dfrac{(l-m)(l-m+1)}{2l+1}c^m_{k,l+1,n}, \end{cases} \tag{6.27}$$

$$c^{m+1}_{k+1,l,n} - c^{m+1}_{k-1,l,n} = \frac{n+m+1}{n-m}(c^m_{k+1,l,n} - c^m_{k-1,l,n})$$
$$+ \frac{2k+1}{2n+1}[(n+m)(n+m+1)c^m_{k,l,n-1} - (n-m)(n-m+1)c^m_{k,l,n+1}]$$
$$= \frac{l+m+1}{l-m}(c^m_{k+1,l,n} - c^m_{k-1,l,n})$$
$$+ \frac{2k+1}{2l+1}[(l+m)(l+m+1)c^m_{k,l-1,n} - (l-m)(l-m+1)c^m_{k,l+1,n}]. \tag{6.28}$$

(6.25) and (6.27) are derived by considering the integrals

$$\int_{-1}^{1} d\mu \cdot \mu P_k(\mu) P_l^m(\mu) P_n^m(\mu)$$

and

$$\int_{-1}^{1} d\mu \, (1 - \mu^2)^{\frac{1}{2}} P_k(\mu) P_l^m(\mu) P_n^{m+1}(\mu),$$

respectively, (6.26) is obtained directly from (6.5), and (6.28) results from (6.29). (6.26) may be used to obtain $c^m_{l+n-2k,l,n}$ by starting with $c^m_{l+n,l,n}$ given in (6.23).

6.3. Recurrence Formulas (6.6) and (6.7)

The calculation of the coefficients c^m_{kln} is a rather tedious work as seen in Sec. 6.2. One who is patient enough to work through the square root of numbers may also be referred to the monographs[12] on Clebsch–Gordon's and Racah's coefficients. He is, however, recommended to deal directly with the functions $J^m_{ln}(x)$ and $H^m_{ln}(x)$ in practical calculations. For the purpose, the recurrence formulas for $J^m_{ln}(x)$, (6.6), and (6.7), may be used most conveniently.

The formulas (6.6) show a way of successive computation of $J^m_{ln}(x)$, $m > 0$, from $J^0_{ln}(x)$'s:

$$J^0_{ln}(x) = \sum_k i^k (2k + 1) c^0_{kln} j_k(x),$$

cf. (6.2), where c^0_{kln} is given by the first expression of (6.21). These $J^0_{ln}(x)$'s could also be computed directly by using (6.7) from

$$J^0_{0n}(x) = i^n j_n(x)$$

and

$$J^0_{1n}(x) = [i^n/(2n + 1)][(n + 1) j_{n+1}(x) - n j_{n-1}(x)]$$

without appealing to the coefficient c^0_{kln}. The explicit forms of the functions $J^0_{ln}(x)$, $l, n \leq 4$, are given in Table II in the Appendix.

The first of the formulas (6.6) is derived by noticing the fact that

$$\int_{-1}^{1} d\mu \frac{\partial}{\partial \mu} [e^{i\mu x} P_l^{(m)}(\mu) P_n^{(-m-1)}(\mu)] = 0,$$

where

$$(-)^{m+1} \frac{(n + m + 1)!}{(n - m - 1)!} [P_l^{(m)}(\mu) P_n^{(-m-1)}(\mu)]$$
$$= P_l^m(\mu) \left[\frac{(n + m)(n + m + 1)}{2n + 1} P_{n-1}^m(\mu) - \frac{(n - m)(n - m + 1)}{2n + 1} P_{n+1}^m(\mu) \right],$$

and that

$$P_l^m(1) = \delta_{m,0}, \qquad P_l^m(-1) = (-)^l \delta_{m,0}.$$

The second equality of (6.6) is a consequence of the symmetry of $J^m_{ln}(x)$ with respect to l and n. Each side of Eq. (6.7) can be shown to be equal to

$$-i(d/dx) J^m_{ln}(x).$$

6.4. Connection with the Delta Function

It may be instructive to note here that an infinite matrix with $J^0_{ln}(x)$ as its (l, n) element has a continuous eigenvalue λ extending from $\exp(-ix)$ to $\exp(ix)$ over the unit circle and that the eigenvalue problem is equivalent to solving an equation

$$(e^{ix\mu} - \lambda) f(\mu) = 0, \qquad -1 \leq \mu \leq 1, \quad x \geq 0,$$

obeyed by a generalized function $f(\mu)$.

We commence with the fact that normalized Ferrers' functions

$$\varphi_l(\mu), \qquad l = m, m + 1, \cdots,$$

where

$$\varphi_l(\mu) = \left[\frac{2l + 1}{2} \frac{(l - m)!}{(l + m)!} \right]^{\frac{1}{2}} P_l^m(\mu), \qquad l \geq m \geq 0,$$

form a complete orthonormal system which spans the Hilbert space consisting all square integrable functions in the closed interval $[-1, +1]$. In fact, we have Vitali's completeness theorem:

$$\sum_{l=m}^{\infty} \left[\int_{\lambda}^{1} d\mu \, \varphi_l(\mu) \right]^2 = 1 - \lambda.$$

Let us consider an infinite matrix $\mathrm{J}(x)$ with parameter x whose (l, n) element is given by

$$\int_{-1}^{1} d\mu \, e^{i\mu x} \varphi_l(\mu) \varphi_n(\mu)$$
$$= \left[(2l + 1)(2n + 1) \frac{(l - m)!}{(l + m)!} \frac{(n - m)!}{(n + m)!} \right]^{\frac{1}{2}} J^m_{ln}(x).$$

Then, the closure property

$$\sum_{l=m}^{\infty} \varphi_l(\lambda) \varphi_l(\mu) = \delta(\lambda - \mu)$$

leads us to a relation

$$\mathrm{J}(x + y) = \mathrm{J}(x) \cdot \mathrm{J}(y),$$

implying that

$$\mathrm{J}(0) = 1, \qquad \mathrm{J}(-x) = [\mathrm{J}(x)]^{-1},$$

and that $\mathrm{J}(x)$ is nonsingular. Since $\mathrm{J}(x)$ is nonsingu-

[12] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957); M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957).

lar, there exists uniquely the matrix $L(x)$ such that

$$J(x) = \exp [L(x)],$$

and that

$$L(x + y) = L(x) + L(y),$$

implying that

$$L(0) = 0 \quad \text{and} \quad L[(n/m)x] = (n/m)L(x),$$

for any pair of natural numbers n and m. Because of the continuity of $J(x)$ and $L(x)$ with respect to x, we deduce that

$$L(x) = ixL, \qquad J(x) = \exp [ixL], \tag{6.29}$$

where

$$L = -iL(1).$$

The (l, n) element of the matrix L is given by

$$\begin{aligned} L_{ln} &= \int_{-1}^{1} d\mu \cdot \mu \varphi_l(\mu)\varphi_n(\mu) \\ &= (2l + 1)^{-\frac{1}{2}}(2n + 1)^{-\frac{1}{2}}[(n^2 - m^2)^{\frac{1}{2}} \\ &\quad \times \delta_{l,n-1} + (l^2 - m^2)^{\frac{1}{2}} \delta_{l-1,n}], \end{aligned} \tag{6.30}$$

which is shown by expanding $J(x)$ in terms of small x and considering the linear term in x.

As can readily be shown, the matrix L has a continuous eigenvalue λ extending from -1 to $+1$ and its associated eigenvector is

$$[\varphi_m(\lambda), \varphi_{m+1}(\lambda), \cdots].$$

It is interesting to trace the passage from a discrete to a continuous spectrum pictorially by starting with an N-dimensional truncated matrix $L^{(N)}$ obtained from L by retaining the first N rows and N columns.

For the sake of simplicity, we assume that $m = 0$ in the following. Let $L_{ln}^{(N)}$ be the (l, n) element of $L^{(N)}$:

$$L_{ln}^{(N)} = \int_{-1}^{1} d\mu \cdot \mu \varphi_l(\mu)\varphi_n(\mu); \quad l, n = 0, 1, \cdots, N - 1,$$

where

$$\varphi_l(\mu) = [\tfrac{1}{2}(2l + 1)]^{\frac{1}{2}} P_l(\mu).$$

Then we have

$$\begin{aligned} \sum_{n=0}^{N-1} L_{ln}^{(N)}\varphi_n(\lambda) &= \lambda\varphi_l(\lambda) - \varphi_N(\lambda) \int_{-1}^{1} d\mu \cdot \mu \varphi_l(\mu)\varphi_N(\mu) \\ &= \lambda\varphi_l(\lambda), \qquad \text{for} \quad l \leq N - 2 \\ &= \lambda\varphi_{N-1}(\lambda) - \frac{N}{(4N^2 - 1)^{\frac{1}{2}}} \varphi_N(\lambda), \\ &\qquad \text{for} \quad l = N - 1. \end{aligned}$$

It is seen that the spectrum of $L^{(N)}$ is constituted by zeros of the Legendre polynomial of degree N, say $\lambda_1^{(N)}, \cdots, \lambda_N^{(N)}$, and that the eigenvector associated with $\lambda_k^{(N)}$ is given by

$$[\varphi_0(\lambda_k^{(N)}), \varphi_1(\lambda_k^{(N)}), \cdots, \varphi_{N-1}(\lambda_k^{(N)})],$$

its length amounting to the square root of

$$\tfrac{1}{2}NP_{N-1}(\lambda_k^{(N)})P_N^{(1)}(\lambda_k^{(N)}),$$

as seen from the Christoffel formula of summation:

$$\sum_{l=0}^{N-1} (2l + 1)P_l(\lambda)P_l(\mu) = NP_{N-1}(\lambda) \frac{P_N(\lambda) - P_N(\mu)}{\lambda - \mu}.$$

The distribution of N zeros of the Legendre polynomial $P_N(\mu)$ is known to be governed by Brun's inequalities:

$$[(k - \tfrac{1}{2})/(N + \tfrac{1}{2})]\pi < \theta_k < [k/(N + \tfrac{1}{2})]\pi,$$

where

$$\theta_k = \cos^{-1} \lambda_k^{(N)}.$$

Hence, the angles $\theta = \cos^{-1}\lambda$ corresponding to the eigenvalues λ tend to be distributed everywhere dense over the semicircle with unit radius as $N \to \infty$ as shown in Fig. 4.

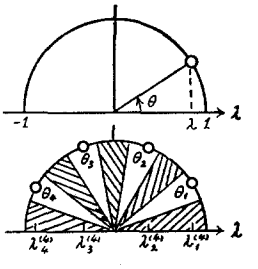

FIG. 4. The distribution of the zeros $\lambda_k^{(4)}$ of Legendre polynomial of order 4. The angles $\theta_k = \cos^{-1} \lambda_k^{(4)}$ corresponding to these zeros are also shown on a semicircle with unit radius.

The eigenvector associated with the continuous spectrum of L is intimately connected with the delta function. Suppose we are given an eigenvalue problem such that

$$\sum_n L_{ln}a_n = \lambda a_n, \tag{6.31}$$

where $(a_0, a_1, a_2, \cdots)$ is an eigenvector with eigenvalue λ. By introducing a function

$$f(x) = \sum_l a_l\varphi_l(x),$$

the problem turns out to be equivalent to that of solving an integral equation

$$\int_{-1}^{1} dx\, \varphi_k(x)(x - \lambda)f(x) = 0; \qquad k = 0, 1, 2, \cdots.$$

This means that

$$\int_{-1}^{1} dx\, \varphi(x)(x - \lambda)f(x) = 0,$$

for any test function $\varphi(x)$ which has a support in the open interval $(-1, +1)$ and has continuous derivatives of arbitrary order. Hence $f(x)$ should obey an equation

$$(x - \lambda)f(x) = 0, \qquad -1 \leq x \leq +1, \qquad (6.32)$$

which implies that the generalized function $f(x)$ is concentrated at the point $x = \lambda$. Such a generalized function should be of the form of a linear combination of the delta function and its derivatives,[13] viz.

$$f(x) = \sum_{k=0}^{m} c_k\, \delta^{(k)}(x - \lambda)$$

with finite m. Further, it is seen that $c_1 = c_2 = \cdots = c_m = 0$, because

$$\int_{-1}^{1} dx\, \varphi(x)(x - \lambda)\, \delta^{(k)}(x - \lambda) = (-)^k k\varphi^{(k-1)}(\lambda),$$

which cannot vanish in general for $k > 0$. Thus we have the solution

$$f(x) = \delta(x - \lambda),$$

which is unique except for a constant factor c_0. At the same time, we have solved the original eigenvalue problem for L, (6.31), and obtained the eigenvector

$$[\varphi_0(\lambda), \varphi_1(\lambda), \varphi_2(\lambda), \cdots]$$

with the eigenvalue λ extending continuously from -1 to $+1$.

The above consideration applies also to a general function F(L) of L. Suppose an analytic function F(z) of z is given by a Taylor series

$$\mathrm{F}(z) = \sum_{n=0}^{\infty} b_n z^n, \qquad |z| < r,$$

with $r > 1$ as its radius of convergence. Then F(L) may be defined, since the characteristic roots of L lie in the circle of convergence of F(z). The whole argument in the last paragraph holds for the matrix F(L) in place of L. Naturally, (6.32) has to be replaced by

$$[\mathrm{F}(\mu) - \lambda]f(\mu) = 0, \qquad -1 \leq \mu \leq +1. \qquad (6.33)$$

This has a nontrivial solution $f(\mu)$ only for such λ that $\lambda = \mathrm{F}(\mu_0)$ for some μ_0 in $[-1, +1]$. The characteristic solution is given by

$$f(\mu) = \delta(\mu - \mu_0)$$

with the characteristic value $\mathrm{F}(\mu_0)$, $-1 \leq \mu_0 \leq 1$. The statement at the beginning of the section concerns with the case where

$$\mathrm{F}(\mu_0) = \exp(ix\mu_0), \qquad -1 \leq \mu_0 \leq 1.$$

7. METHOD OF DIVERGENT INTEGRALS

So far, the deduction has been developed within the scope of the classical analysis except for that in Sec. 6.4. A short cut in the procedure can be made, however, if we do not hesitate to make use of divergent integrals to be understood as generalized functions. Concerning the theory of generalized functions as applied to differential operators, the reader may be referred to Hörmander.[14]

Consider, as an example, an integral

$$\int_0^{\infty} dr\, r^2 j_l(r) j_l(kr) = \tfrac{1}{2}\pi k^{l-1}[\delta(k - 1) + \delta(k + 1)]. \qquad (7.1)$$

Although it scarcely has any meaning in the classical analysis because of the divergence at $r = \infty$, cf. (2.13), we may understand it as the generalized function given on the right.

The proof follows from Sonine's integral[15]

$$\int_0^{\infty} dr \cdot r^{\mu-\lambda+1} J_\lambda(r) J_\mu(kr) = \frac{k^\mu (1 - k^2)_+^{\lambda-\mu-1}}{2^{\lambda-\mu-1}\Gamma(\lambda - \mu)}, \qquad R(\lambda - \mu) > 0, \qquad (7.2)$$

where $(1 - k^2)_+^z$ denotes the discontinuous function given by

$$(1 - k^2)_+^z = \begin{cases} (1 - k^2)^z, & \text{when } 1 - k^2 > 0, \\ 0, & \text{when } 1 - k^2 \leq 0. \end{cases}$$

The integral (7.2) is written in terms of spherical Bessel functions in the form

$$\int_0^{\infty} dr\, r^{l-\lambda+2} j_\lambda(r) j_l(kr) = \frac{\pi k^l (1 - k^2)_+^{\lambda-l-1}}{2^{\lambda-l}\Gamma(\lambda - l)}, \qquad (7.3)$$

where l is a fixed positive integer. Since the generalized function $(1 - k^2)_+^{z-1}$ has simple poles with residues

$$(-)^n\, \delta^{(n)}(1 - k^2)/n!$$

[13] I. M. Gel'fand and G. E. Schilow, *Verallgemeinerte Funktionen, I* (VEB Deutscher Verlag der Wissenschaften, Berlin, 1960).

[14] L. Hörmander, *Linear Partial Differential Operators* (Springer-Verlag, Berlin, 1963).

[15] For example, I. N. Sneddon, *Fourier Transforms* (McGraw-Hill Book Company, Inc., New York, 1951).

at $z = -n$, $n = 0, 1, 2, \cdots$, and the gamma function $\Gamma(z)$ has also simple poles with residues

$$(-)^n/n!,$$

we have

$$\frac{2^{l-\lambda}k^l(1-k^2)_+^{\lambda-l-1}}{\Gamma(\lambda-l)} \to k^l\,\delta(1-k^2), \quad \text{as} \quad \lambda \to l.$$

Applying, further, a general formula

$$\delta(f(x)) = \sum_n \frac{1}{|f'(x_n)|}\,\delta(x-x_n), \tag{7.4}$$

which is valid for an infinitely differentiable function $f(x)$ with only simple zeros at $x = x_n$, $n = 1, 2, \cdots$. Then, the proof of (7.1) is completed.

In virtue of the integral (7.1), the Fourier transform of the Helmholtz' solid harmonic $J_l^m(\mathbf{r})$ is obtained immediately. In fact, defining the Fourier transform $F(\mathbf{k})$ of a function $f(\mathbf{r})$ by

$$F(\mathbf{k}) = (2\pi)^{-3}\int d\mathbf{r}\,\exp(-i\mathbf{kr})f(\mathbf{r}), \tag{7.5}$$

we have, for $f(\mathbf{r}) = J_l^m(\mathbf{r})$,

$$\begin{aligned} F(\mathbf{k}) &= (2\pi^2)^{-1}P_l^m(\mu_k)e^{im\varphi_k}\int_0^\infty dr\,r^2 j_l(r)j_l(kr) \\ &= (4\pi)^{-1}k^{l-1}\,\delta(k-1)P_l^m(\mu_k)e^{im\varphi_k}, \qquad 0 \le k, \end{aligned} \tag{7.6}$$

where $(k, \cos^{-1}\mu_k, \varphi_k)$ is the polar coordinate corresponding to $\mathbf{k}$.

The differential operator (3.2) generating $J_l^m(\mathbf{r})$, $m \ge 0$, is obtained in the process of Fourier inversion:

$$\begin{aligned} J_l^m(\mathbf{r}) &= (-i)^m(4\pi)^{-1}\int d\mathbf{k}\,k^{-1}\,\delta(k-1) \\ &\quad\cdot[ik(1-\mu_k^2)^{\frac{1}{2}}e^{i\varphi_k}]^m P_l^{(m)}(k\mu_k)e^{i\mathbf{kr}} \\ &= (-i)^m\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)^m P_l^{(m)}\left(-i\frac{\partial}{\partial z}\right)(4\pi)^{-1} \\ &\quad\cdot\int d\mathbf{k}\,k^{-1}\,\delta(k-1)e^{i\mathbf{kr}} \\ &= (-i)^m\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)^m P_l^{(m)}\left(-i\frac{\partial}{\partial z}\right)j_0(r), \end{aligned}$$

where the second equality comes from the identity

$$\mathbf{kr} = k(1-\mu_k^2)^{\frac{1}{2}}\cos\varphi_k\cdot x + k(1-\mu_k^2)^{\frac{1}{2}}\sin\varphi_k\cdot y + \mu_k\cdot z.$$

Similarly, we have, for $m \ge 0$,

$$\begin{aligned} J_l^{-m}(\mathbf{r}) &= i^m\frac{(l-m)!}{(l+m)!}(4\pi)^{-1}\int d\mathbf{k}\,k^{-1}\,\delta(k-1) \\ &\quad\cdot(ik(1-\mu_k^2)^{\frac{1}{2}}e^{-i\varphi_k})^m P_l^{(m)}(k\mu_k)e^{i\mathbf{kr}}, \\ &= i^m\frac{(l-m)!}{(l+m)!}\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)^m P_l^{(m)}\left(-i\frac{\partial}{\partial z}\right)j_0(r). \end{aligned}$$

The addition theorem (4.1) may also be derived readily from the inversion formula

$$f(\mathbf{r}) = \int d\mathbf{k}\,\exp(i\mathbf{kd})\,\exp(i\mathbf{kr}')F(\mathbf{k}),$$

where $\mathbf{r} = \mathbf{d} + \mathbf{r}'$, Fig. 2. In fact, substitution of (7.6) yields

$$\begin{aligned} &J_l^m(\mathbf{r}) \\ &= \frac{1}{2}\int_0^\infty dk\,k^{l+1}\,\delta(k-1)\int_{-1}^1 d\mu_k\,P_l^m(\mu_k)e^{ikd\mu_k} \\ &\quad\times\sum_{n=|m|}^\infty(2n+1)(-)^m J_n^m(k\mathbf{r}')P_n^{-m}(\mu_k) \\ &= \sum_{n=|m|}^\infty(2n+1)J_n^m(\mathbf{r}')(-)^m\int_{-1}^1 d\mu\,e^{i\mu d}P_l^m(\mu)P_n^{-m}(\mu) \\ &= \frac{(l+m)!}{(l-m)!}\sum_{n=|m|}^\infty(2n+1)J_n^m(\mathbf{r}')J_{ln}^{-m}(d). \end{aligned}$$

8. DISCUSSION

One of the most important applications of the bipolar expansion formula is the evaluation of two-center integrals especially in quantum chemistry. The main advantage of the bipolar expansion formula lies in the fact that it allows us to perform angular integrations around two centers independently of radial integrations.

Unfortunately, however, this is true only for the following three cases:

(i) $r < d$ and $r' < d$;
(ii) $r + d < r'$;
(iii) $r' + d < r$.

For the overlapping case

(iv) $|r - r'| < d < r + r'$,

μ or μ' integration cannot be done over the complete range -1 to $+1$, as pointed out by Buehler and Hirschfelder.[3] The trouble comes essentially from the presence of singularity of the screened (or usual) Coulomb potential $e^{-\alpha R}/R$ in the overlapping region (iv).

A remedy to surmount the difficulty is furnished by the method of Fourier transform. Let us consider a screened Coulomb integral with two centers O and O′, as shown in Fig. 1,

$$V = \int d\mathrm{P}\int d\mathrm{P}'\,\rho(\mathrm{P})\frac{e^{-\alpha R}}{R}\rho'(\mathrm{P}'), \tag{8.1}$$

where $\rho(\mathrm{P})$ and $\rho'(\mathrm{P})$ are given density distributions around the centers O and O′, respectively,

$$\rho(\mathrm{P}) = \sum_l \sum_m \rho_{lm}(r) P_l^m(\mu) e^{im\varphi};$$
$$\rho'(\mathrm{P}') = \sum_n \sum_m \rho'_{nm}(r') P_l^m(\mu') e^{im\varphi'}. \tag{8.2}$$

Then, we can derive a formula

$$V = 32\pi \sum_l \sum_n \sum_m i^{n-l}(-)^m \frac{(n-m)!}{(n+m)!} \times \int_0^\infty dk \frac{k^2}{k^2+\alpha^2} J_{ln}^m(kd) j\rho_{lm}(k) j\rho'_{n,-m}(k), \tag{8.3}$$

where $J_{ln}^m(x)$ is the function defined by (4.3) and investigated in detail in Sec. 6 and

$$\left.\begin{matrix} j\rho_{lm}(k) \\ j\rho'_{lm}(k) \end{matrix}\right\} = \int_0^\infty dr \cdot r^2 j_l(kr) \begin{cases} \rho_{lm}(r) \\ \rho'_{lm}(r). \end{cases} \tag{8.4}$$

It is seen that the singularity of the screened Coulomb potential has been integrated out in the formula (8.3). The detail of the Fourier transform method has been published in Sec. 8 of Preprint No. 759 by the Quantum Chemistry Group, Uppsala University, Uppsala, Sweden, which is available on request.

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TABLE I. Numerical values of the coefficients c^0_{kln}:

$$c^0_{kln} = \frac{1}{2}\int_{-1}^{1} d\mu\, P_k(\mu) P_l(\mu) P_n(\mu), \qquad \text{cf.} \quad (6.21),$$

which are given in the table in the order of increasing $g = \frac{1}{2}(k+l+n)$. The superscripts zeros are deleted for brevity.

$c_{011} = \frac{1}{3}$, $c_{022} = \frac{1}{5}$, $c_{112} = \frac{2}{3\cdot 5}$,

$c_{033} = \frac{1}{7}$, $c_{123} = \frac{3}{5\cdot 7}$, $c_{222} = \frac{2}{5\cdot 7}$,

$c_{044} = \frac{1}{9}$, $c_{134} = \frac{4}{7\cdot 9}$, $c_{224} = \frac{2}{5\cdot 7!}$, $c_{233} = \frac{4}{3\cdot 5\cdot 7}$,

$c_{055} = \frac{1}{11}$, $c_{145} = \frac{5}{9\cdot 11}$, $c_{235} = \frac{10}{3\cdot 7\cdot 11}$,

$c_{244} = \frac{20}{7\cdot 9\cdot 11}$, $c_{334} = \frac{2}{7\cdot 11}$,

$c_{066} = \frac{1}{13}$, $c_{156} = \frac{6}{11\cdot 13}$, $c_{246} = \frac{5}{11\cdot 13}$, $c_{255} = \frac{10}{3\cdot 11\cdot 13}$,

$c_{336} = \frac{100}{3\cdot 7\cdot 11\cdot 13}$, $c_{345} = \frac{20}{7\cdot 11\cdot 13}$, $c_{444} = \frac{18}{7\cdot 11\cdot 13}$,

$c_{077} = \frac{1}{15}$, $c_{167} = \frac{7}{13\cdot 15}$, $c_{257} = \frac{21}{5\cdot 11\cdot 13}$, $c_{266} = \frac{14}{5\cdot 11\cdot 13}$,

$c_{347} = \frac{35}{9\cdot 11\cdot 13}$, $c_{356} = \frac{7}{3\cdot 11\cdot 13}$, $c_{446} = \frac{5}{3\cdot 11\cdot 13}$, $c_{455} = \frac{2}{11\cdot 13}$,

$c_{088} = \frac{1}{17}$, $c_{178} = \frac{8}{15\cdot 17}$, $c_{268} = \frac{28}{5\cdot 13\cdot 17}$, $c_{277} = \frac{56}{13\cdot 15\cdot 17}$,

$c_{358} = \frac{56}{11\cdot 13\cdot 17}$, $c_{367} = \frac{168}{5\cdot 11\cdot 13\cdot 17}$, $c_{448} = \frac{490}{9\cdot 11\cdot 13\cdot 17}$,

$c_{457} = \frac{280}{9\cdot 11\cdot 13\cdot 17}$, $c_{466} = \frac{28}{11\cdot 13\cdot 17}$, $c_{556} = \frac{80}{3\cdot 11\cdot 13\cdot 17}$.

TABLE II. Explicit forms of the functions $J^0_{ln}(x)$:

$$J^0_{ln}(x) = \frac{1}{2}\int_{-1}^{1} d\mu\, e^{i\mu x} P_l(\mu) P_n(\mu) = \sum_{k=|l-n|}^{l+n} i^k (2k+1) c_{kln} j_k(x)$$

J_{ln} and j_k stand for $J^0_{ln}(x)$ and $j_k(x)$, respectively; cf. (4.3), (6.29), and (6.30).

$$J_{00} = j_0, \qquad J_{01} = i\cdot j_1, \qquad J_{02} = -j_2, \qquad J_{03} = -i\cdot j_3,$$

$$J_{11} = \frac{1}{3} j_0 - \frac{2}{3} j_2, \qquad J_{12} = i\left(\frac{2}{5} j_1 - \frac{3}{5} j_3\right), \qquad J_{22} = \frac{1}{5} j_0 - \frac{2}{7} j_2 + \frac{18}{35} j_4,$$

$$J_{13} = -\frac{3}{7} j_2 + \frac{4}{7} j_4, \qquad J_{23} = i\left(\frac{9}{35} j_1 - \frac{4}{15} j_3 + \frac{10}{21} j_5\right),$$

$$J_{33} = \frac{1}{7} j_0 - \frac{4}{21} j_2 + \frac{18}{77} j_4 - \frac{100}{231} j_6, \qquad J_{14} = i\left(-\frac{4}{9} j_3 + \frac{5}{9} j_5\right),$$

$$J_{24} = -\frac{2}{7} j_2 + \frac{20}{7\cdot 11} j_4 - \frac{5}{11} j_6, \qquad J_{34} = i\left(\frac{4}{3\cdot 7} j_1 - \frac{2}{11} j_3 + \frac{20}{7\cdot 13} j_5 - \frac{175}{3\cdot 11\cdot 13} j_7\right),$$

$$J_{44} = \frac{1}{9} j_0 - \frac{100}{7\cdot 9\cdot 11} j_2 + \frac{162}{7\cdot 11\cdot 13} j_4 - \frac{5}{3\cdot 11} j_6 + \frac{490}{9\cdot 11\cdot 13} j_8.$$

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APPENDIX I

Three tables are given here. Table I shows numerical values of the coefficients c^0_{kln}, from which we could obtain the values of c^m_{kln} according to the formulas (6.25) to (6.28). Table II gives explicit expressions for the functions $J^0_{ln}(x)$ with l and $n \leq 4$. Those for $J^m_{ln}(x)$, $m \geq 1$, may be obtained using the formulas (6.6) to (6.7). Table III is a list of spherical Bessel, Neumann, and Hankel functions of lowest integral orders.

APPENDIX II

It may be of help to scientists working in the field to summarize useful theorems and formulas for spherical Bessel functions which are scattered in the literature. Since the collection of them is rather lengthy, it will be published as a Technical Note from the Quantum Chemistry Group, Uppsala, Sweden.

In that Technical Note, the spherical Bessel function $j_\lambda(z)$ of complex order λ and with complex argument z is defined by

$$j_\lambda(z) = \frac{z^\lambda}{2^{\lambda+1}\Gamma(\lambda+1)} \int_{-1}^{1} dt \exp(izt)\cdot(1-t^2)^\lambda$$

based on the recurrence formulas

$$\begin{cases} (2\lambda+1)\dfrac{1}{z} j_\lambda(z) = j_{\lambda-1}(z) + j_{\lambda+1}(z), \\ (2\lambda+1)\dfrac{d}{dz} j_\lambda(z) = \lambda j_{\lambda-1}(z) - (\lambda+1) j_{\lambda+1}(z). \end{cases} \tag{A1}$$

The theory of spherical Bessel functions is not a special case of the theory of Bessel functions unless we confine ourselves to those of integral orders. They are logically equivalent to each other.

Here, an elementary proof is given of the orthogonality of $j_l(x)$'s:

$$\int_{-\infty}^{\infty} dt\, j_l(t) j_n(t) = \frac{\pi}{2l+1}\delta_{ln}. \tag{A2}$$

Proof: Replace the j_l's by their integral representations (2.6) and perform the t integration. Then the integral is written in the form

$$\frac{2\pi}{4i^{l+n}} \int_{-1}^{1} d\lambda \int_{-1}^{1} d\mu\, P_l(\lambda) P_l(\mu)\, \delta(\lambda+\mu)$$

$$= \frac{2\pi(-)^l}{4i^{l+n}} \int_{-1}^{1} d\mu\, P_l(\mu) P_n(\mu),$$

$$= \frac{\pi}{2l+1}\delta_{ln}, \qquad \text{Q.E.D.}$$

TABLE III. Spherical Bessel functions of integral order.

$$j_0(x) = \frac{\sin x}{x},$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x},$$

$$j_2(x) = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x,$$

$$j_3(x) = \left(\frac{15}{x^4} - \frac{6}{x^2}\right)\sin x - \left(\frac{15}{x^3} - \frac{1}{x}\right)\cos x,$$

$$j_4(x) = \left(\frac{105}{x^5} - \frac{45}{x^3} + \frac{1}{x}\right)\sin x - \left(\frac{105}{x^4} - \frac{10}{x^2}\right)\cos x,$$

$$j_5(x) = \left(\frac{945}{x^6} - \frac{420}{x^4} + \frac{15}{x^2}\right)\sin x - \left(\frac{945}{x^5} - \frac{105}{x^3} + \frac{1}{x}\right)\cos x$$

$$n_0(x) = -\frac{\cos x}{x},$$

$$n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x},$$

$$n_2(x) = -\left(\frac{3}{x^3} - \frac{1}{x}\right)\cos x - \frac{3}{x^2}\sin x,$$

$$n_3(x) = -\left(\frac{15}{x^4} - \frac{6}{x^2}\right)\cos x - \left(\frac{15}{x^3} - \frac{1}{x}\right)\sin x,$$

$$n_4(x) = -\left(\frac{105}{x^5} - \frac{45}{x^3} + \frac{1}{x}\right)\cos x - \left(\frac{105}{x^4} - \frac{10}{x^2}\right)\sin x,$$

$$n_5(x) = -\left(\frac{945}{x^6} - \frac{420}{x^4} + \frac{15}{x^2}\right)\cos x - \left(\frac{945}{x^5} - \frac{105}{x^3} + \frac{1}{x}\right)\sin x,$$

$$h_0(x) = -\frac{i}{x}e^{ix},$$

$$h_1(x) = \left(-\frac{1}{x} - \frac{i}{x^2}\right)e^{ix},$$

$$h_2(x) = \left(\frac{i}{x} - \frac{3}{x^2} - \frac{i\cdot 3}{x^3}\right)e^{ix},$$

$$i_0(x) = \frac{e^x - e^{-x}}{2x},$$

$$i_1(x) = \frac{1}{2}\left(\frac{1}{x} - \frac{1}{x^2}\right)e^x + \frac{1}{2}\left(\frac{1}{x} + \frac{1}{x^2}\right)e^{-x},$$

$$i_2(x) = \frac{1}{2}\left(\frac{1}{x} - \frac{3}{x^2} + \frac{3}{x^3}\right)e^x - \frac{1}{2}\left(\frac{1}{x} + \frac{3}{x^2} + \frac{3}{x^3}\right)e^{-x},$$

$$k_0(x) = \frac{1}{x}e^{-x},$$

$$k_1(x) = -\left(\frac{1}{x} + \frac{1}{x^2}\right)e^{-x},$$

$$k_2(x) = \left(\frac{1}{x} + \frac{3}{x^2} + \frac{3}{x^3}\right)e^{-x}.$$

Discrete Degenerate Representations of Noncompact Rotation Groups. I

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The discrete most degenerate principal series of irreducible Hermitian representations of the Lie algebra of an arbitrary noncompact as well as compact rotation group $SO(p, q)$ are derived. The properties of these representations are discussed and the explicit form of the corresponding harmonic functions is given.

1. INTRODUCTION

PROPERTIES of representations of a semisimple Lie group are closely related to the properties of its Cartan subgroup. That is, the number of different principal series of irreducible unitary representations is equal to the number of nonisomorphic Cartan subgroups of a considered semisimple Lie group.[1] Moreover, if a given Cartan subgroup is isomorphic to a direct product of a k-dimensional linear space and an r-dimensional torus, then there exists a corresponding series of irreducible unitary representations determined by k real numbers and r integers.[1] Hence, if a semisimple Lie group has a compact Cartan subgroup, then there exists a discrete principal series of irreducible unitary representations characterized only by integers.

The number N of nonisomorphic Cartan subgroups contained in an arbitrary noncompact rotation group $SO(p, q)$ is enumerated in Table I.

We see that there is a discrete nondegenerate principal series of irreducible unitary representations in classes (i), (ii), and (iii). However, we show that the most degenerate principal series exists even in the class (iv). Of course, besides the principal series, there also exist supplementary series, which we do not consider. Their existence is closely related to the existence of a double-point measure.[2]

The discrete principal series of irreducible unitary representations of the $SO(p, q)$ group have been constructed only in special cases: for the Lorentz groups[3] $SO(2, 1)$ and $SO(3, 1)$, for the $SO(2, 2)$ group,[4] and for the de Sitter groups[5] $SO(4, 1)$ and $SO(3, 2)$.[6] In the present work, we consider the properties of the discrete most degenerate principal series of irreducible unitary single-valued representations for an arbitrary $SO(p, q)$ group.[7] We restrict ourselves to the discrete most degenerate principal series of representations, since these representations seem to be of great importance in quantum mechanics and in elementary-particle physics.

The main idea behind our construction method of the most degenerate representations of $SO(p, q)$ groups is explained in Sec. 2. In Sec. 3, the properties of the discrete most degenerate representations of $SO(p, q)$ groups for $p \geq q > 2$ are discussed and the explicit form of harmonic functions is given. The properties of the discrete degenerate representations of the $SO(p, 2)$ groups, $p \geq 2$, are considered in Sec. 4. It is shown that there are three principal series of discrete most degenerate representations in this case. Section 5 contains the construction of the discrete representations of the so-called Lorentz-type groups, i.e., $SO(p, 1)$ groups. In Sec. 6, the proof of irreducibility and unitarity of our representations are presented. In Sec. 7, properties of the derived discrete representations are discussed. Finally, in the Appendix, the most degenerate representations of an arbitrary compact rotation group $SO(p)$ is derived.

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[5] L. H. Thomas, Ann. Math. 42, 113 (1941); T. D. Newton, Ann. Math. 51, 730 (1950); J. Dixmier, Bull. Soc. Math. France 89, 9 (1961).

[6] J. B. Ehrman, Proc. Cambridge Phil. Soc. 53, 290 (1957).

[7] In the following we speak about representations of the group $SO(p, q)$ on the Hilbert space $\mathfrak{H}$, although we derive only representations of the Lie algebra $\mathfrak{R}$ of the considered group on definite vector space $\mathfrak{L}$, which is dense in the Hilbert space $\mathfrak{H}$. However, in paper III of our series of articles it will be shown that our infinitesimal representations induce the global irreducible unitary representations of the group $SO(p, q)$.

2. DISCRETE MOST DEGENERATE REPRESENTATIONS OF $SO(p, q)$ GROUPS

Different principal series of irreducible unitary representations of a semisimple Lie group may be created, in the Hilbert space $\mathfrak{H}(X)$, of functions with the domain X, a homogeneous space of the type

$$X = G/G_0,$$

where G_0 is a closed subgroup of G.[2]

The number of independant invariant operators characterizing different irreducible representations by their eigenvalues is equal to the rank of the space x.[8,9,10] Consequently, the most degenerate representations, determined by one invariant operator, are representations in the Hilbert space of functions whose domain is a homogeneous space of rank one.

In a homogeneous space of rank one, the invariant operator is just the Laplace–Beltrami operator of the form[11]

$$\Delta(X) = [\bar{g}(X)]^{-\frac{1}{2}}\,\partial_\alpha\, g^{\alpha\beta}(X)[\bar{g}(X)]^{\frac{1}{2}}\,\partial_\beta, \qquad (2.1)$$

where $g_{\alpha\beta}(X)$ is the left-invariant metric tensor on X and $\bar{g}(X) = |\det [g_{\alpha\beta}(X)]|$.[12]

If the metric tensor $g_{\alpha\beta}(X)$ on X is induced by the Cartan metric tensor g_{ik} in the Lie algebra R of the group G, then the Laplace–Beltrami operator $\Delta(X)$ is equal to the second-order Casimir operator $Q_2 = g_{ik}X^iX^k$ (see Chap. X, Sec. 7 of Ref. 9). Thus, the construction of most degenerate irreducible unitary representations may be reduced to the following:

(i) Construction of a convenient coordinate system on X, in which the metric tensor $g_{\alpha\beta}(X)$ is diagonal.

TABLE I. Nonisomorphic Cartan subgroups in $SO(p, q)$.

Class	p	q	N	Compact Cartan subgroup
(i)	even	even	$\frac{1}{2}[\min(p, q)] + 1$	yes
(ii)	even	odd	$\min(p, q) + 1$	yes
(iii)	odd	even	$\min(p, q) + 1$	yes
(iv)	odd	odd	$\frac{1}{2}[\min(p, q)] + 1$	no

(ii) Solution of the eigenvalue problem for the Laplace–Beltrami operator

$$\Delta(X)\cdot\psi_\lambda = \lambda\cdot\psi_\lambda.$$

(iii) Proof of the irreducibility and unitarity of the representations related to a set of harmonic functions ψ_λ.

For homogeneous spaces X, we may take the quotient spaces G/G_0 with a compact or noncompact stability group G_0. The homogeneous spaces of rank k with the compact stability group related to $SO(p, q)$ groups are[13]

$$X_k = SO_0(p, q)/SO_0(p) \times SO_0(q).$$

Since the rank k of these Cartan symmetric spaces is equal to $\min(p, q)$, we may construct in these spaces the most degenerate representation only of the Lorentz-type groups $SO(p, 1)$. For an arbitrary $SO(p, q)$ group, we have to consider more general spaces of rank one. We may take these spaces as homogeneous spaces of rank one of the following form:

$$\text{and} \quad \begin{aligned} X_+^{p+q-1} &= SO_0(p, q)/SO_0(p-1, q), \\ X_-^{p+q-1} &= SO_0(p, q)/SO_0(p, q-1), \end{aligned} \qquad (2.2)$$

where superscript $p + q - 1$ denotes the dimension of the space $X_\pm^{p+q-1}$.[14]

3. DISCRETE MOST DEGENERATE REPRESENTATIONS OF $SO(p, q)$ GROUPS ($p \geq q > 2$)

To choose a suitable coordinate system, we have to introduce some convenient model of the space $X_\pm^{p+q-1}$ in (2.2). This means that we have to introduce a manifold, with the same dimension and the same stability group as $X_\pm^{p+q-1}$ itself and on which the group $SO(p, q)$ acts transitively.

For the space X_+^{p+q-1}, such a model can be realized by the hyperboloid H_q^p determined by the equation

$$(x^1)^2 + \cdots + (x^p)^2 - (x^{p+1})^2 - \cdots - (x^{p+q})^2 = 1. \qquad (3.1)$$

As an appropriate model for the space X_-^{p+q-1}, we take the hyperboloid H_p^q defined by the equation

$$(x^1)^2 + \cdots + (x^q)^2 - (x^{q+1})^2 - \cdots - (x^{q+p})^2 = 1. \qquad (3.2)$$

[8] I. M. Gel'fand, Transl. Am. Math. Soc., Ser. 2, **37**, 31 (1964).

[9] S. Helgason, *Differential Geometry and Symmetric Spaces* (Academic Press Inc., New York, 1962), Chap. X.

[10] I. M. Gel'fand and M. I. Graev, Tr. Mosk. Mat. Obshch. **8**, 321 (1959).

[11] In fact this theorem has been proved for the space X being Euclidean or a global symmetric one of rank 1 (Ref. 9, Chap. X, §2). However, we may extend it on homogeneous spaces of rank 1 by using results of Gel'fand and Graev of Ref. 10.

[12] If no other indication is given, we employ the Einstein summation convention.

[13] See Ref. 9, Chap. IX. $SO_0(a, b)$ denotes a component continuously connected with the identity of the group $SO(a, b)$.

[14] Such spaces were classified by B. A. Rosenfeld, Dokl. Akad. Nauk SSSR **110**, 23 (1956).

If we introduce internal coordinates $\Omega = \{\theta^1, \cdots, \theta^{p+q-1}\}$ on the space H_q^p(or H_p^q) (which is imbedded in the flat Minkowski space $M^{p,q}$), then the metric tensor $g_{\alpha\beta}(H_q^p)$ on the hyperboloid H_q^p is induced by the metric tensor $g_{ab}(M^{p,q})$ on the Minkowski space $M^{p,q}$, and is defined as

$$g_{\alpha\beta}(H_q^p) = g_{ab}(M^{p,q}) \cdot \partial_\alpha x^a(\Omega) \cdot \partial_\beta x^b(\Omega), \qquad (3.3)$$

where $a, b = 1, 2, \cdots, p + q$ and $\alpha, \beta = 1, 2, \cdots, p + q - 1$.

Generally, we may choose a large number of different coordinate systems on the hyperboloid H_q^p (or H_p^q), in which the Laplace–Beltrami operator can be separated. However, as follows from our previous work,[15] the most convenient coordinate system is the biharmonic one, because, in this system, the maximal Abelian compact subalgebra of the considered $SO(p, q)$ group is automatically contained in the maximal set of commuting operators.

The biharmonic coordinate system on the hyperboloid H_q^p (3, 1) is constructed as follows:

$$\begin{aligned} x^k &= x'^k \cosh\theta, \quad k = 1, 2, \cdots, p, \quad \theta \in [0, \infty), \\ x^{p+l} &= \hat{x}^l \sinh\theta, \quad l = 1, 2, \cdots, q, \end{aligned} \qquad (3.4)$$

where the form of the x'^k and $\hat{x}^l$ depends on whether p and q are even or odd. We must distinguish four cases:

$$\begin{aligned} &\text{(i)} \quad p = 2r; \qquad q = 2s, \\ &\text{(ii)} \quad p = 2r; \qquad q = 2s + 1, \\ &\text{(iii)} \quad p = 2r + 1; \quad q = 2s, \\ &\text{(iv)} \quad p = 2r + 1; \quad q = 2s + 1, \end{aligned} \qquad r, s = 1, 2, \cdots. \qquad (3.5)$$

Then, if p is even ($p = 2r$), the corresponding $x'^k (k = 1, 2, \cdots, 2r)$ are given by the recursion formulas

$$\begin{aligned} \text{for } r = 1 \qquad x'^1 &= \cos\varphi^1, & \varphi^1 &\in [0, 2\pi), \\ x'^2 &= \sin\varphi^1, & & \\ \text{for } r > 1 \qquad x'^i &= x''^i \sin\vartheta^r, & i &= 1, 2, \cdots, 2r - 2, \\ x'^{2r-1} &= \cos\varphi^r \cos\vartheta^r, & \varphi^j &\in [0, 2\pi), \quad j = 1, 2, \cdots, r, \\ x'^{2r} &= \sin\varphi^r \cos\vartheta^r, & \vartheta^k &\in [0, \tfrac{1}{2}\pi], \quad k = 2, 3, \cdots, r, \end{aligned} \qquad (3.6)$$

and, if p is odd ($p = 2r + 1$), we first construct the x^{*i}, $i = 1, 2, \cdots, 2r$, by using the above-mentioned method for $p = 2r$; we then obtain the corresponding x'^k, $k = 1, 2, \cdots, 2r + 1$, as

$$\begin{aligned} x'^i &= x^{*i} \sin\vartheta^{r+1}, \quad i = 1, 2, \cdots, 2r, \\ x'^{2r+1} &= \cos\vartheta^{r+1}, \quad \vartheta^{r+1} \in [0, \pi]. \end{aligned} \qquad (3.7)$$

The recursion formulas for $\hat{x}^l$, q, even or odd, are the same as those for x'^k, p, even or odd, respectively, except that angles φ^i, ϑ^j in x'^k are replaced by $\tilde{\varphi}^i$, $\tilde{\vartheta}^j$.

Choosing the parametrization $\Omega \equiv \{\omega, \tilde{\omega}, \theta\}$ on the hyperboloid H_q^p as[16]

$$\begin{aligned} \omega &\equiv \{\varphi^1, \cdots, \varphi^{[\frac{1}{2}p]}, \vartheta^2, \cdots, \vartheta^{[\frac{1}{2}p]}\}, \\ \tilde{\omega} &\equiv \{\tilde{\varphi}^1, \cdots, \tilde{\varphi}^{[\frac{1}{2}q]}, \tilde{\vartheta}^2, \cdots, \tilde{\vartheta}^{[\frac{1}{2}q]}\}, \end{aligned} \qquad (3.8)$$

and denoting

$$\{\partial_\gamma\} \equiv \left\{\frac{\partial}{\partial\varphi^1}, \frac{\partial}{\partial\vartheta^2}, \cdots, \frac{\partial}{\partial\varphi^{[\frac{1}{2}p]}}, \frac{\partial}{\partial\vartheta^{[\frac{1}{2}p]}}, \frac{\partial}{\partial\tilde{\varphi}^1}, \frac{\partial}{\partial\tilde{\varphi}^1}, \frac{\partial}{\partial\tilde{\vartheta}^2}, \cdots, \frac{\partial}{\partial\tilde{\varphi}^{[\frac{1}{2}q]}}, \frac{\partial}{\partial\tilde{\vartheta}^{[\frac{1}{2}q]}}, \frac{\partial}{\partial\theta}\right\},$$

$$\gamma = 1, 2, \cdots, p + q - 1, \qquad (3.9)$$

we can calculate the metric tensor $g_{\alpha\beta}(H_q^p)$ as well as the Laplace–Beltrami operator $\Delta(H_q^p)$.

Since in all four cases of (3.5) the variables in the Laplace–Beltrami operator (2.1) are separated in the

[15] J. Niederle and R. Raczka, International Centre for Theoretical Physics, preprint IC/65/89, Trieste (1965).

[16] Here and elsewhere, we use brackets for indices defined as follows:

$$[\tfrac{1}{2}a] = \begin{cases} \tfrac{1}{2}a & \text{if } a = 2r \\ \tfrac{1}{2}(a-1) & \text{if } a = 2r+1 \end{cases}, \qquad \{\tfrac{1}{2}a\} = \begin{cases} \tfrac{1}{2}a & \text{if } a = 2r \\ \tfrac{1}{2}(a+1) & \text{if } a = 2r+1 \end{cases}, \qquad r = 1, 2, \cdots.$$

same way due to properties of the metric tensor (3.3), we can write the operator $\Delta(H_q^p)$ in the form

$$\Delta(H_q^p) = -(\cosh^{p-1}\theta \sinh^{q-1}\theta)^{-1}\frac{\partial}{\partial\theta}\cosh^{p-1}\theta\sinh^{q-1}\theta\frac{\partial}{\partial\theta} + \frac{\Delta(S^{p-1})}{\cosh^2\theta} - \frac{\Delta(S^{q-1})}{\sinh^2\theta}, \tag{3.10}$$

where $\Delta(S^{p-1})[\Delta(S^{q-1})]$ is the Laplace–Beltrami operator of the rotation group $SO(p)[SO(q)]$.[17] If we represent the eigenfunctions of $\Delta(H_q^p)$ as a product of the eigenfunctions of $\Delta(S^{p-1})$, $\Delta(S^{q-1})$, and a function $\psi^{\lambda}_{l_{(p/2)},l_{(q/2)}}(\theta)$, we obtain the following equation:

$$\left[-(\cosh^{p-1}\theta\sinh^{q-1}\theta)^{-1}\cdot\frac{d}{d\theta}\cosh^{p-1}\theta\sinh^{q-1}\theta\cdot\frac{d}{d\theta} - \frac{l_{(\frac{1}{2}p)}(l_{(\frac{1}{2}p)}+p-2)}{\cosh^2\theta} + \frac{\bar{l}_{(\frac{1}{2}q)}(\bar{l}_{(\frac{1}{2}q)}+q-2)}{\sinh^2\theta} - \lambda\right]\cdot\psi^{\lambda}_{l_{(p/2)},l_{(q/2)}}(\theta) = 0, \tag{3.11}$$

where $l_{(\frac{1}{2}p)}(l_{(\frac{1}{2}p)}+p-2)[\bar{l}_{(\frac{1}{2}q)}(\bar{l}_{(\frac{1}{2}q)}+q-2)]$ are eigenvalues of the operator $\Delta(S^{p-1})[\Delta(S^{q-1})]$ with $l_{(\frac{1}{2}p)}[\bar{l}_{(\frac{1}{2}q)}]$ the certain nonnegative integers for $p > 2$ $[q > 2]$.

A discrete series of representations exist if there exist solutions of (3.11), which are square integrable functions $\psi^{\lambda}_{l_{(p/2)},l_{(q/2)}}(\theta)$, $(\theta) \in (0, \infty)$, with respect to the measure[18]

$$d\mu(\theta) = \cosh^{p-1}\theta\cdot\sinh^{q-1}\theta\cdot d\theta, \tag{3.12}$$

which is induced by the measure[18] $d\mu(\Omega)$ on the hyperboloid H_q^p:

$$d\mu(\Omega) = [\bar{g}(H_q^p)]^{\frac{1}{2}}\,d\Omega = d\mu(\omega)\,d\mu(\tilde{\omega})\cosh^{p-1}\theta\sinh^{q-1}\theta\,d\theta. \tag{3.13}$$

The left-invariant measure $d\mu(\omega)$ is defined in (A8). Since the differential equation (3.11) has meromorphic coefficients regular in the interval $(0, \infty)$, any two linearly independent solutions are also regular analytic in this interval.[19] Since at the origin and at infinity the coefficients are singular, the solutions are not generally regular there, and we can easily find two essentially distinct behaviors of the solutions at the origin: $\psi_1^0 \sim \theta^{l_{(p/2)}}$,

$$\psi_2^0 \sim \theta^{-l_{(q/2)}-q+2},$$

and at infinity:

$$\psi_{1,2}^{\infty} \sim \exp\{-\tfrac{1}{2}(p+q-2) \pm \{[\tfrac{1}{2}(p+q-2)]^2 - \lambda\}^{\frac{1}{2}}\}\theta.$$

The only satisfactory solution, i.e., the solution square-integrable with respect to our measure $d\mu(\theta)$ (3.12), is the one that behaves like $\psi_1^0(\theta)$ at the origin and like $\psi_2^{\infty}(\theta)$ at infinity. It turns out that the solution of (3.11) with these properties is

$$\psi^{\lambda}_{l_{(p/2)},l_{(q/2)}}(\theta) = \tanh^{l_{(q/2)}}\theta\cdot\cosh^{-\{\frac{1}{2}(p+q-2)+[\frac{1}{2}(p+q-2)^2-\lambda]^{\frac{1}{2}}\}}\theta \cdot {}_2F_1\left(-n + l_{(\tfrac{1}{2}p)} + \frac{p-2}{2}, -n; \bar{l}_{(\tfrac{1}{2}q)} + \frac{q}{2}; \tanh^2\theta\right),$$

where a nonnegative integer n is connected with $l_{(\frac{1}{2}p)}$, $\bar{l}_{(\frac{1}{2}q)}$, and λ by the condition that ${}_2F_1$ be a polynomial, i.e.,

$$l_{(\frac{1}{2}p)} - \bar{l}_{(\frac{1}{2}q)} - 2n = \tfrac{1}{2}(p+q-2) + \{[\tfrac{1}{2}(p+q-2)]^2 - \lambda\}^{\frac{1}{2}} - p + 2, \qquad n = 0, 1, 2, \cdots. \tag{3.14}$$

From this restrictive condition, we can find that the discrete spectrum of the operator $\Delta(H_q^p)$ is of the form[16]

$$\lambda = -L(L+p+q-2), \qquad L = -\{\tfrac{1}{2}(p+q-4)\}, -\{\tfrac{1}{2}(p+q-4)\}+1, \cdots, \tag{3.15}$$

where

$$L = l_{(\frac{1}{2}p)} - \bar{l}_{(\frac{1}{2}q)} - q - 2n. \tag{3.16}$$

Thus we have shown that there exist discrete most degenerate series of representations of an arbitrary $SO(p, q)$ group $(p \geq q > 2)$ on the Hilbert space $\mathfrak{H}^L(H_q^p)$, i.e., on the space of square-integrable functions

[17] For more details, see the Appendix.

[18] The measure $d\mu(\Omega) = [\bar{g}(H_q^p)]^{1/2}\,d\Omega$ is the Riemannian measure, which is left invariant under the action of $SO(p, q)$ on H_q^p, See Ref. 9.

[19] E. L. Ince, *Ordinary Differential Equations* (Dover Publications, Inc., New York, 1956).

$\psi^{\lambda, l_2, \cdots, l_{[p/2]}; \tilde{l}_2, \cdots, \tilde{l}_{[q/2]}}_{m_1, \cdots, m_{[p/2]}; \tilde{m}_1, \cdots, \tilde{m}_{[q/2]}}(\omega, \tilde{\omega}, \theta)$ with respect to the measure $d\mu(\Omega)$ (3.13) and with λ given in (3.15). We denote such a series of representations by $D^L(H^p_q)$.

The basis of the Hilbert space $\mathfrak{H}^L(H^p_q)$ is formed by the orthonormal functions:

$$Y^{L, l_2, \cdots, l_{[p/2]}; \tilde{l}_2, \cdots, \tilde{l}_{[q/2]}}_{m_1, \cdots, m_{[p/2]}; \tilde{m}_1, \cdots, \tilde{m}_{[q/2]}}(\omega, \tilde{\omega}, \theta) = Y^{l_2, \cdots, l_{[p/2]}}_{m_1, \cdots, m_{[p/2]}}(\omega) \cdot Y^{\tilde{l}_2, \cdots, \tilde{l}_{[q/2]}}_{\tilde{m}_1, \cdots, \tilde{m}_{[q/2]}}(\tilde{\omega}) \cdot V^L_{l_{[p/2]}, \tilde{l}_{[q/2]}}(\theta), \tag{3.17}$$

where

$$Y^{l_2, \cdots, l_{[p/2]}}_{m_1, \cdots, m_{[p/2]}}(\omega) \equiv \begin{cases} Y^{l_2, \cdots, l_r}_{m_1, \cdots, m_r}(\omega) = (N_r^{-\frac{1}{2}}) \prod_{k=2}^{r} \sin^{2-k}(\vartheta^k) \cdot d^{J_k}_{M_k; M_k}(2\vartheta^k) \cdot \prod_{k=1}^{r} \exp i m_k \varphi^k, & \text{if } p = 2r, \\ Y^{l_2, \cdots, l_{r+1}}_{m_1, \cdots, m_r}(\omega) = (N_{r+1}^{-\frac{1}{2}}) \sin^{1-r}(\vartheta^{r+1}) \cdot d^{J_{r+1}}_{M_{r+1}; 0}(\vartheta^{r+1}) & \\ \quad \cdot \prod_{k=2}^{r} \sin^{2-k}(\vartheta^k) \cdot d^{J_k}_{M_k; M_k}(2\vartheta^k) \cdot \prod_{k=1}^{r} \exp i m_k \varphi^k, & \text{if } p = 2r+1, \end{cases} \tag{3.18}$$

are eigenfunctions of $\Delta(S^{p-1})$ derived in the Appendix; $Y^{\tilde{l}_2, \cdots, \tilde{l}_{[q/2]}}_{\tilde{m}_1, \cdots, \tilde{m}_{[q/2]}}(\tilde{\omega})$ are eigenfunctions of $\Delta(S^{q-1})$ expressed as the product of the usual d-functions of angular momenta and exponential functions exactly as (3.18), but respectively of variables $\tilde{\varphi}^i$, $\tilde{\vartheta}^i$, and $\tilde{l}_k$, $\tilde{m}_l$ instead of φ^i, ϑ^i, and l_k, m_l; and $V^L_{l_{[p/2]}, \tilde{l}_{[q/2]}}$ is the solution of (3.11) given by

$$V^L_{l_{[p/2]}, \tilde{l}_{[q/2]}}(\theta) = (N^{-\frac{1}{2}}) \cdot \tanh^{\tilde{l}_{[q/2]}}(\theta) \cdot \cosh^{-(L+p+q-2)}(\theta)$$
$$\cdot {}_2F_1[\tfrac{1}{2}(p + q - 2 + l_{[\frac{1}{2}p]} + \tilde{l}_{[\frac{1}{2}q]} + L), \tfrac{1}{2}(L + q + \tilde{l}_{[\frac{1}{2}q]} - l_{[\frac{1}{2}p]}); \tilde{l}_{[\frac{1}{2}q]} + \tfrac{1}{2}q; \tanh^2\theta], \tag{3.19}$$

where, for a definite representation, L is fixed and $l_{[\frac{1}{2}p]}$, $\tilde{l}_{[\frac{1}{2}q]}$ are restricted by the condition that ${}_2F_1$ be a polynomial, i.e.,

$$l_{[\frac{1}{2}p]} - \tilde{l}_{[\frac{1}{2}q]} = L + q + 2n, \qquad n = 0, 1, 2, \cdots. \tag{3.20}$$

N_r, N_{r+1}, N are normalization factors given by

$$N_r = 2\pi^r \prod_{k=2}^{r} (l_k + k - 1)^{-1}, \qquad N_{r+1} = 4\pi^r [2(l_{r+1} + r) - 1]^{-1} \prod_{k=2}^{r} (l_k + k - 1)^{-1}, \tag{3.21}$$

$$N = \frac{\Gamma[\frac{1}{2}(l_{[\frac{1}{2}p]} - \tilde{l}_{[\frac{1}{2}q]} - L - q + 2)]\Gamma^2\left(\tilde{l}_{[\frac{1}{2}q]} + \frac{q}{2}\right)\Gamma[\frac{1}{2}(L - \tilde{l}_{[\frac{1}{2}q]} + l_{[\frac{1}{2}p]} + p)]}{2[L + \frac{1}{2}(p + q - 2)]\Gamma[\frac{1}{2}(l_{[\frac{1}{2}p]} + \tilde{l}_{[\frac{1}{2}q]} + L + p + q - 2)]\Gamma[\frac{1}{2}(l_{[\frac{1}{2}p]} + \tilde{l}_{[\frac{1}{2}q]} - L)]} \tag{3.22}$$

and the indices J_k, M_k, M'_k are defined as:

$$\begin{aligned} J_k &= \tfrac{1}{2}(l_k + k - 2), \\ M_k &= \tfrac{1}{2}(m_k + l_{k-1} + k - 2), \qquad l_1 \equiv m_1 \\ M'_k &= \tfrac{1}{2}(m_k - l_{k-1} - k + 2), \text{ for } k = 2, 3, \cdots, r. \\ J_{r+1} &= l_{r+1} + r - 1, \; M_{r+1} = l_r + r - 1, \end{aligned} \tag{3.23}$$

l_k, $k = 2, \cdots, r+1$, are nonnegative integers, m_k, $k = 1, \cdots, r$, are integers restricted as follows (See Appendix):

$$\begin{aligned} |m_2| + |m_1| &= l_2 - 2n_2, \\ |m_3| + l_2 &= l_3 - 2n_3, \cdots, |m_r| + l_{r-1} = l_r - 2n_r, \\ n_k &= 0, 1, \cdots, \{\tfrac{1}{2}l_k\}, \\ l_r = l_{r+1} - n_{r+1}, \qquad k &= 2, 3, \cdots, r, \\ n_{r+1} &= 0, 1, \cdots, l_{r+1}. \end{aligned} \tag{3.24}$$

There exists also a discrete series of representations $D^L(H^q_p)$ on the Hilbert space $\mathfrak{H}^L(H^q_p)$ with H^q_p given in (3.2). This series is obtained formally from the previous $D^L(H^p_q)$ by exchanging p, $l_{[\frac{1}{2}p]}$ for q, $\tilde{l}_{[\frac{1}{2}q]}$, respectively, and vice versa. The most degenerate representations $D^L(H^q_p)$ created on $\mathfrak{H}^L(H^q_p)$ are not unitarily equivalent except in the case $p = q$, when both Hilbert spaces coincide.

Finally, we would like to mention that the representations $D^L(H^p_q)$ and $D^L(H^q_p)$ are irreducible and unitary, as will be proved in Sec. 6.

4. DISCRETE MOST DEGENERATE REPRESENTATIONS OF $SO(p, 2)$ GROUPS ($p \geq 2$)

For the de Sitter-type groups, $SO(p, 2)$, the homogeneous spaces are

$$\begin{aligned} X^{p+1}_+ &= SO_0(p, 2)/SO_0(p-1, 2), \\ \text{and} \qquad X^{p+1}_- &= SO_0(p, 2)/SO_0(p, 1), \end{aligned} \tag{4.1}$$

and can be represented, respectively, by hyperboloids H^2_2 and H^2_p.

The biharmonic coordinate system is introduced again in the same way as in Sec. 3. Hence, for the Laplace–Beltrami operator $\Delta(H_p^2)$ we obtain

$$\Delta(H_p^2) = -(\cosh\theta \sinh^{p-1}\theta)^{-1}\frac{\partial}{\partial\theta}\cosh\theta\sinh^{p-1}\theta\frac{\partial}{\partial\theta} + (\cosh^2\theta)^{-1}\frac{\partial^2}{(\partial\tilde{\varphi}^1)^2} - \frac{\Delta(S^{p-1})}{\sinh^2\theta}. \tag{4.2}$$

The main difference with respect to the equation for $\Delta(H_p^2)$ is rooted in the fact that instead of the operator $\Delta(S^{q-1})$, $q > 2$, appearing in equation (4.2), the operator $\Delta(S^1) = \partial^2/(\partial\tilde{\alpha}^1)^2$, which has eigenvalues $-(\tilde{m}_1)^2$ with $\tilde{m}_1$ an arbitrary integer appears. By using the same procedure as in Sec. 3, we finally obtain, for the function of θ, the equation:

$$\left[-(\cosh\theta\sinh^{p-1}\theta)^{-1}\frac{d}{d\theta}\cosh\theta\sinh^{p-1}\theta\frac{d}{d\theta} - \frac{(\tilde{m}_1)^2}{\cosh^2\theta} + \frac{l_{(\frac{1}{2}p)}(l_{(\frac{1}{2}p)}+p-2)}{\sinh^2\theta} - \lambda\right]\psi^{\lambda}_{\tilde{m}_1,l_{(p/2)}}(\theta) = 0. \tag{4.3}$$

The discrete series of representations exist, again due to the fact that there exist solutions of (4.3) square integrable in $\theta \in (0, \infty)$ with respect to the measure $d\mu(\theta) = \sinh^{p-1}\theta\cdot\cosh\theta\cdot d\theta$.

The discrete spectrum of the operator $\Delta(H_p^2)$ looks like

$$\lambda = -L(L+p),$$
$$L = -\{\tfrac{1}{2}(p-2)\}, -\{\tfrac{1}{2}(p-2)\}+1, \cdots, \tag{4.4}$$

where

$$L = |\tilde{m}_1| - |l_{(\frac{1}{2}p)}| - 2n - p. \tag{4.5}$$

In a definite representation, the value L is fixed and Eq. (4.5) imposes the following restriction on $|\tilde{m}_1|$:

$$|\tilde{m}_1| \geq L + p. \tag{4.6}$$

Since generators of an $SO(p, q)$ group can change the quantum number $\tilde{m}_1$ only by one (see Sec. 6), we create on $\mathfrak{K}^L(H_p^2)$ two discrete unitarily nonequivalent series of representations. The representation corresponding to $\tilde{m}_1 \geq L + p$ is denoted by $D_+^L(H_2^p)$, and the other corresponding to $\tilde{m}_1 \leq -(L+p)$ is denoted by $D_-^L(H_p^2)$.

The representations $D_\pm^L(H_p^2)$ are representations on different invariant subspaces of the Hilbert space $\mathfrak{K}^L(H_p^2)$, with basis formed by the following orthonormal functions

$$Y^{L,l_2,\cdots,l_{[p/2]}}_{m_1,\cdots,m_{[p/2]},\tilde{m}_1}(\omega,\tilde{\varphi}^1,\theta) = Y^{l_2,\cdots,l_{[p/2]}}_{m_1,\cdots,m_{[p/2]}}(\omega)[(2\pi)^{-\frac{1}{2}}\exp i\tilde{m}_1\tilde{\varphi}^1]V^L_{\tilde{m}_1,l_{(p/2)}}(\theta), \tag{4.7}$$

where $Y^{l_2,\cdots,l_{[p/2]}}_{m_1,\cdots,m_{[p/2]}}$ is given in (3.18) and

$$V^L_{\tilde{m}_1,l_{(p/2)}}(\theta) = (N^{-\frac{1}{2}})\tanh^{|l_{(p/2)}|}\theta\cdot\cosh^{-(L+p)}\theta \cdot {}_2F_1[\tfrac{1}{2}(-|\tilde{m}_1| + |l_{(\frac{1}{2}p)}| + L + p), \tfrac{1}{2}(|\tilde{m}_1| + |l_{(\frac{1}{2}p)}| + L + p); |l_{(\frac{1}{2}p)}| + \tfrac{1}{2}p; \tanh^2\theta],$$
$$N = \frac{\Gamma^{\frac{1}{2}}(|\tilde{m}_1| - |l_{(\frac{1}{2}p)}| - L - p + 2)\Gamma^2(|l_{(\frac{1}{2}p)}| + \frac{1}{2}p)\Gamma^{\frac{1}{2}}(L - |l_{(\frac{1}{2}p)}| + |\tilde{m}_1| + 2)}{2(L+\frac{1}{2}p)\Gamma^{\frac{1}{2}}(|\tilde{m}_1| + |l_{(\frac{1}{2}p)}| + L + p)\Gamma^{\frac{1}{2}}(|\tilde{m}_1| + |l_{(\frac{1}{2}p)}| - L)}, \tag{4.8}$$

where, for a definite representation, L is fixed and $\tilde{m}_1$, $l_{(\frac{1}{2}p)}$ are restricted by the condition that ${}_2F_1$ be a polynomial, i.e.,

$$|\tilde{m}_1| - |l_{(\frac{1}{2}p)}| = L + p + 2n, \quad n = 0, 1, \cdots. \tag{4.9}$$

The discrete series of representations on the Hilbert space $\mathfrak{K}^L(H_2^p)$ are constructed by the same method, but (except $p = 2$) we obtain only one series because now $l_{(\frac{1}{2}p)}$ plays the role of $\tilde{m}_1$; and, for $p > 2$, $l_{(\frac{1}{2}p)}$ is a nonnegative integer. For $p = 2(l_1 \equiv m_1)$, we find again two discrete unitarily nonequivalent series as both Hilbert spaces $\mathfrak{K}^L(H_p^2)$ and $\mathfrak{K}^L(H_2^p)$ coincide.

5. DISCRETE MOST DEGENERATE REPRESENTATIONS OF $SO(p, 1)$ GROUPS

The homogeneous spaces of rank one for the Lorentz-type groups are

$$\text{and} \qquad X_+^p = SO_0(p,1)/SO_0(p-1,1), \qquad X_-^p = SO_0(p,1)/SO_0(p), \tag{5.1}$$

where the X_-^p space is the Cartan symmetric one. We take, respectively, the hyperboloids H_1^p and H_p^1 as their models.

The biharmonic coordinates on H_1^p and H_p^1 are introduced again by the method explained in Sec. 3, but, on the hyperboloid H_1^p, the range of θ is $(-\infty, \infty)$. On the hyperboloid H_p^1, the range of θ

is from zero to infinity since we restrict ourselves to the upper sheet of the hyperboloid H_p^1. Of course, the upper sheet of H_p^1 is a transitive manifold only under the proper $SO_0(p, 1)$ group, i.e., under the group of transformations $g = (g_{ik})$, for which g_{11} is positive.

The Laplace–Beltrami operator on the Hilbert space $\mathfrak{H}(H_1^p)$ has the form

$$\Delta(H_1^p) = \frac{-1}{\cosh^{p-1}\theta}\frac{\partial}{\partial\theta}\cosh^{p-1}\theta\frac{\partial}{\partial\theta} + \frac{\Delta(S^{p-1})}{\cosh^2\theta}, \qquad \theta \in (-\infty, \infty), \tag{5.2}$$

where $\Delta(S^{p-1})$ is the Laplace–Beltrami operator for the $SO(p)$ group given in the Appendix.

The eigenvalue problem of $\Delta(H_1^p)$ is reduced to

$$\left[\frac{-1}{\cosh^{p-1}\theta}\frac{d}{d\theta}\cosh^{p-1}\theta\frac{d}{d\theta} - \frac{l_{(\frac{1}{2}p)}(l_{(\frac{1}{2}p)}+p-2)}{\cosh^2\theta} - \lambda\right]\psi^{\lambda}_{l_{(p/2)}}(\theta) = 0. \tag{5.3}$$

Analogous to the previous cases, we find the discrete spectrum of $\Delta(H_1^p)$ to be of the form

$$\lambda = -L(L+p-1),$$
$$L = -\{\tfrac{1}{2}(p-3)\}, -\{\tfrac{1}{2}(p-3)\}+1, \cdots, \tag{5.4}$$

where

$$L = |l_{(\frac{1}{2}p)}| - 1 - n, \tag{5.5}$$

$l_{(\frac{1}{2}p)}$ a positive integer for $p > 2$, and, for $p = 2$, an arbitrary nonzero integer, m_1. Hence, there is an exceptional case for $p = 2$ and we again obtain two types of discrete unitarily nonequivalent series of representations $D_+^L(H_1^2)$ and $D_-^L(H_1^2)$ on different invariant subspaces of the Hilbert space $\mathfrak{H}^L(H_1^2)$. For $SO(2, 1)$ and $SO(3, 1)$ these results were obtained by Bargmann,[3] and for $SO(4, 1)$ by Dixmier.[5]

The basis of the Hilbert space $\mathfrak{H}^L(H_1^p)$ is formed by the orthonormal functions

$$Y^{L,l_2,\cdots,l_{(p/2)}}_{m_1,\cdots,m_{(p/2)}}(\omega,\theta) = \begin{cases} {}_1Y^{L,l_2,\cdots,l_{(p/2)}}_{m_1,\cdots,m_{(p/2)}}(\omega,\theta) = Y^{l_2,\cdots,l_{(p/2)}}_{m_1,\cdots,m_{(p/2)}}(\omega)\cdot{}_1V^L_{l_{(p/2)}}(\theta), & \text{if } L - l_{(\frac{1}{2}p)} = -(2n+2), \\ {}_2Y^{L,l_2,\cdots,l_{(p/2)}}_{m_1,\cdots,m_{(p/2)}}(\omega,\theta) = Y^{l_2,\cdots,l_{(p/2)}}_{m_1,\cdots,m_{(p/2)}}(\omega)\cdot{}_2V^L_{l_{(p/2)}}(\theta), & \\ \qquad\qquad \text{if } L - l_{(\frac{1}{2}p)} = -(2n+1), \quad n = 0, 1, 2, \cdots, & \end{cases} \tag{5.6}$$

where $Y^{l_2,\cdots,l_{(p/2)}}_{m_1,\cdots,m_{(p/2)}}(w)$ is explicitly given in Eq. (3.18) and

$$\begin{aligned} {}_1V^L_{l_{(p/2)}}(\theta) &= -2({}_1N^{-\frac{1}{2}})\tanh\theta\cdot\cosh^{-(L+p-1)}\theta\cdot{}_2F_1[\tfrac{1}{2}(L+l_{(\frac{1}{2}p)}+p), \tfrac{1}{2}(L-l_{(\frac{1}{2}p)}+2); \tfrac{3}{2}; \tanh^2\theta]. \\ {}_2V^L_{l_{(p/2)}}(\theta) &= ({}_1N^{-\frac{1}{2}})\cosh^{-(L+p-1)}\theta\cdot{}_2F_1[\tfrac{1}{2}(L+l_{(\frac{1}{2}p)}+p-1), \tfrac{1}{2}(L-l_{(\frac{1}{2}p)}+1); \tfrac{1}{2}; \tanh^2\theta]. \end{aligned} \tag{5.7}$$

Here, the normalization factors ${}_1N$, ${}_2N$ are of the form

$$\begin{aligned} {}_1N &= 2\pi\{\Gamma[\tfrac{1}{2}(l-L)]\cdot\Gamma[\tfrac{1}{2}(l+L+p-1)]\}\{[2L+p-1]\cdot\Gamma[\tfrac{1}{2}(l+L+p)]\cdot\Gamma[\tfrac{1}{2}(l-L+1)]\}^{-1} \\ {}_2N &= \{\pi\Gamma[\tfrac{1}{2}(l_{(\frac{1}{2}p)}-L+1)]\Gamma[\tfrac{1}{2}(l_{(\frac{1}{2}p)}+L+p)]\} \\ &\quad\times\{[L+\tfrac{1}{2}(p-1)]\Gamma[\tfrac{1}{2}(l_{(\frac{1}{2}p)}+L+p-1)]\Gamma[\tfrac{1}{2}(l_{(\frac{1}{2}p)}-L)]\}^{-1} \end{aligned} \tag{5.8}$$

and, for a definite representation, L is fixed and $l_{(p/2)}$ must satisfy the restrictive condition that ${}_2F_1$ be a polynomial, i.e.,

$$|l_{(\frac{1}{2}p)}| = L + 1 + n, \qquad n = 0, 1, 2, \cdots. \tag{5.9}$$

The discrete series of representations on the Hilbert space $\mathfrak{H}^L(H_p^1)$ does not exist, because the Laplace–Beltrami operator

$$\Delta(H_p^1) = -(\sinh^{p-1}\theta)^{-1}\frac{d}{d\theta}\sinh^{p-1}\theta\frac{d}{d\theta} - \frac{l_{(\frac{1}{2}p)}(l_{(\frac{1}{2}p)}+p-2)}{\sinh^2\theta},$$

$\theta \in [0, \infty)$, has no discrete spectrum.

6. IRREDUCIBILITY AND UNITARITY

The Lie algebra R of the group $SO(p, q)$ can be expressed in the form of two types of operators with commutation relations:

$$\begin{aligned} &[L_{ij}, L_{rs}]_- \\ &\quad = -\delta_{ir}L_{js} + \delta_{is}L_{jr} + \delta_{jr}L_{is} - \delta_{js}L_{ir}, \\ &[L_{ij}, B_{rs}]_- \\ &\quad = -\delta_{ir}B_{js} - \delta_{is}B_{jr} + \delta_{jr}B_{is} + \delta_{js}B_{ir}, \\ &[B_{ij}, B_{rs}]_- \\ &\quad = \delta_{ir}L_{js} + \delta_{is}L_{jr} + \delta_{jr}L_{is} + \delta_{js}L_{ir}, \end{aligned} \tag{6.1}$$

where L_{ij} and B_{ij} are, respectively, the generators of the compact and noncompact one-parameter

subgroups. We represent the Lie algebra R on the linear manifold $\mathfrak{L}$ composed of the set of harmonic functions

$$Y^{L,l_2,\cdots,l_{[p/2]},l_2,\cdots,l_{[q/2]}}_{m_1,\cdots,m_{[p/2]},\tilde{m}_1,\cdots,\tilde{m}_{[q/2]}}(\omega, \tilde{\omega}, \theta)$$

by the Lie algebra of operators:

$$L_{ij} = \left[x^i\left(\frac{\partial\varphi^1}{\partial x^j}\right) - x^j\left(\frac{\partial\varphi^1}{\partial x^i}\right)\right]\frac{\partial}{\partial\varphi^1} + \cdots + \left[x^i\left(\frac{\partial\vartheta^{([p/2])}}{\partial x^j}\right) - x^j\left(\frac{\partial\vartheta^{([p/2])}}{\partial x^i}\right)\right]\frac{\partial}{\partial\vartheta^{([p/2])}}, \qquad (6.2)$$

where $i, j = 1, 2, \cdots, p$ and $x^1, \cdots, x^p$ are defined by (3.4). For the remaining operators L_{ij}, $i, j = p + 1, p + 2, \cdots, p + q$, we obtain analogous expressions. The generators of the noncompact type are represented by:

$$B_{ij} = \frac{x^i x^j}{\sinh\theta\cosh\theta}\frac{\partial}{\partial\theta} + x^i\left(\frac{\partial\varphi^1}{\partial x^j}\right)\frac{\partial}{\partial\varphi^1} + \cdots + x^i\left(\frac{\partial\vartheta^{([p/2])}}{\partial x^j}\right)\frac{\partial}{\partial\vartheta^{([p/2])}} + x^i\left(\frac{\partial\tilde{\varphi}^1}{\partial x^j}\right)\frac{\partial}{\partial\tilde{\varphi}^1} + \cdots + x^i\left(\frac{\partial\tilde{\vartheta}^{([q/2])}}{\partial x^j}\right)\frac{\partial}{\partial\tilde{\vartheta}^{([q/2])}}, \qquad (6.3)$$

where $i = 1, 2, \cdots, p$ and $j = p + 1, p + 2, \cdots, p + q$. It turns out that the differential operators L_{ij} do not contain derivatives with respect to θ; and their coefficients depend, respectively, only on the parameters ω or $\tilde{\omega}$ of the corresponding subgroup. The differential operators B_{ij} contain the derivative with respect to θ and their coefficients generally depend on all of the parameters ω, $\tilde{\omega}$, and θ.

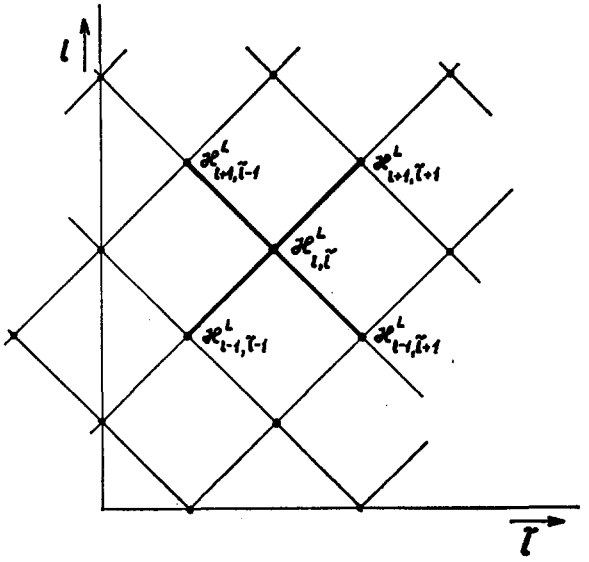

FIG. 1.

A. Irreducibility

To prove the irreducibility of our representations $D^L(H^p_q)$ on the Hilbert space $\mathfrak{HC}^L(H^p_q)$, we show that there is no invariant subspace of the space $\mathfrak{HC}^L(H^p_q)$ with respect to the representation (6.2), (6.3) of the Lie algebra R.

(a) The Case $p \geq q > 2$

The Hilbert space $\mathfrak{HC}^L(H^p_q)$ has the structure

$$\mathfrak{HC}^L(H^p_q) = \sum_{l_{([p/2])},\tilde{l}_{([q/2])}} \oplus \mathfrak{HC}^L_{l_{([p/2])},\tilde{l}_{([q/2])}}(H^p_q), \qquad (6.4)$$

where the sum is taken over all such nonnegative integers $l_{([\frac{1}{2}p])}$, $\tilde{l}_{([\frac{1}{2}q])}$, which satisfy $l_{([\frac{1}{2}p])} - \tilde{l}_{([\frac{1}{2}q])} - 2n = L + q$, $n = 0, 1, 2, \cdots$.
Here the subspaces

$$\mathfrak{HC}^L_{l_{([p/2])},\tilde{l}_{([q/2])}}(H^p_q)$$

are the finite-dimensional spaces spanned by all the harmonic functions (3.17) with fixed values of pairs of integers $l_{([\frac{1}{2}p])}$, $\tilde{l}_{([\frac{1}{2}q])}$. The representation (6.2) of the algebra of the maximal compact subgroup $SO(p) \times SO(q)$ is irreducible on the space

$$\mathfrak{HC}^L_{l_{([p/2])},\tilde{l}_{([q/2])}}(H^p_q)$$

(as is proved in the Appendix). The structure of the Hilbert space $\mathfrak{HC}^L(H^p_q)$ can be graphically illustrated by use of nets. A characteristic detail of the net is drawn in Fig. 1. Every node of the net represents a subspace

$$\mathfrak{HC}^L_{l_{([p/2])},\tilde{l}_{([q/2])}}(H^p_q),$$

and every unit step in the net connects the two nearest neighboring subspaces.

Thus, to prove that there is no invariant subspace of the space $\mathfrak{HC}^L(H^p_q)$ with respect to the operators in (6.2) and (6.3), it is sufficient to find one operator B_{ij} and one element

$$Y^{L,l_{([p/2])},\tilde{l}_{([q/2])}} \in \mathfrak{HC}^L_{l_{([p/2])},\tilde{l}_{([q/2])}}(H^p_q)$$

such that

$$BY^{L,l_{([p/2])},\tilde{l}_{([q/2])}}$$

has nonvanishing components in four neighboring subspaces (see Fig. 1).

Let us show that

$$B_{p,p+q}Y^{L,l_{([p/2])},\tilde{l}_{([q/2])}}_{m_{([p/2])},\tilde{m}_{([q/2])}}(\Omega)$$

has the desired properties if

$$Y^{L,l_{([p/2])},\tilde{l}_{([q/2])}}_{m_{([p/2])},m_{([q/2])}}(\Omega) \equiv Y^{L,l_2,\cdots,l_{([p/2])},\tilde{l}_2,\cdots,\tilde{l}_{([q/2])}}_{m_1,\cdots,m_{([p/2])},\tilde{m}_1,\cdots,\tilde{m}_{([q/2])}}(\Omega),$$

where $m_2 = \cdots = m_{([\frac{1}{2}p])} = \tilde{m}_2 = \cdots = \tilde{m}_{([\frac{1}{2}q])} = 0$, and $m_1, l_2, \cdots, l_{([\frac{1}{2}p])-1}, \tilde{m}_1, \tilde{l}_2, \cdots, \tilde{l}_{([\frac{1}{2}q])-1}$ have the

minimal possible values. Omitting indices $\{\frac{1}{2}p\}$, $\{\frac{1}{2}q\}$ whenever such omission does not lead to misunderstanding, we obtain the following expression:

$$
\begin{aligned}
(BY^{L,l,\tilde{l}}_{0,0})(\Omega) = &-\frac{(\tilde{l}+l+L+p+q-2)(\tilde{l}+l-L)}{2\tilde{l}+q} A_+(l)A_+(\tilde{l})\left[\frac{N(l+1,\tilde{l}+1)}{N(l,\tilde{l})}\right]^{\frac{1}{2}} Z^{L,l+1,\tilde{l}+1}(\Omega) \\
&+ (2\tilde{l}+q-2)A_+(l)A_-(\tilde{l})\left[\frac{N(l+1,\tilde{l}-1)}{N(l,\tilde{l})}\right]^{\frac{1}{2}} Z^{L,l+1,\tilde{l}-1}(\Omega) \\
&- \frac{(\tilde{l}-l+L+q)(\tilde{l}-l-L-p+2)}{2\tilde{l}+q} A_-(l)A_+(\tilde{l})\left[\frac{N(l-1,\tilde{l}+1)}{N(l,\tilde{l})}\right]^{\frac{1}{2}} Z^{L,l-1,\tilde{l}+1}(\Omega) \\
&+ (2\tilde{l}+q-2)A_-(l)A_-(\tilde{l})\left[\frac{N(l-1,\tilde{l}-1)}{N(l,\tilde{l})}\right]^{\frac{1}{2}} Z^{L,l-1,\tilde{l}-1}(\Omega), \qquad (6.5)
\end{aligned}
$$

where

$$
Z^{L,l_{(\frac{1}{2}p)},\tilde{l}_{(\frac{1}{2}q)}}(\Omega) = \begin{cases} Y^{L,l_{r+1},\tilde{l}_{s+1}}_{0,0}(\Omega), & \text{if } \begin{matrix} p=2r+1, \\ q=2s+1, \end{matrix} \\ (2i)^{-1}[Y^{L,l_r,\tilde{l}_{s+1}}_{1,0}(\Omega) - Y^{L,l_r,\tilde{l}_{s+1}}_{-1,0}(\Omega)], & \text{if } \begin{matrix} p=2r, \\ q=2s+1, \end{matrix} \\ -\frac{1}{4}Y^{L,l_r,\tilde{l}_s}_{1,1}(\Omega) + \frac{1}{4}Y^{L,l_r,\tilde{l}_s}_{1,-1}(\Omega) + \frac{1}{4}Y^{L,l_r,\tilde{l}_s}_{-1,1}(\Omega) - \frac{1}{4}Y^{L,l_r,\tilde{l}_s}_{-1,-1}(\Omega), & \text{if } \begin{matrix} p=2r, \\ q=2s, \end{matrix} \end{cases}
$$

$$
r, s = 1, 2, \cdots . \qquad (6.6)
$$

Here $N(l_{(\frac{1}{2}p)}, \tilde{l}_{(\frac{1}{2}q)}) = N_{(\frac{1}{2}p)}, N_{(\frac{1}{2}q)}, N$, where $N_{(\frac{1}{2}p)}$, $N_{(\frac{1}{2}q)}$, and N are defined by the expressions (3.21) and (3.22). Then, if p is even:

$$
\begin{aligned}
&p = 2r \quad r = 2, 3, \cdots \\
&A_\pm(l_{(\frac{1}{2}p)}) \equiv A_\pm(l_r) \\
&= C(J_r, \tfrac{1}{2}, J_r \pm \tfrac{1}{2}, M_r, \tfrac{1}{2}) \cdot C(J_r, \tfrac{1}{2}, J_r \pm \tfrac{1}{2}, -M_r, \tfrac{1}{2}); \qquad (6.7)
\end{aligned}
$$

and, if p is odd, then

$$
\begin{aligned}
&p = 2r+1 \qquad r = 1, 2, \cdots \\
&A_\pm(l_{(\frac{1}{2}p)}) \equiv A_\pm(l_{r+1}) \\
&= C(J_{r+1}, 1, J_{r+1} \pm 1, M_{r+1}, 0) \\
&\cdot C(J_{r+1}, 1, J_{r+1} \pm 1, 0, 0), \qquad (6.8)
\end{aligned}
$$

where the Clebsch–Gordan coefficients $C(J_1, l, J_2, m_1, m_2)$ are taken from Ref. 20, and $J_{(\frac{1}{2}p)}$, $M_{(\frac{1}{2}p)}$ are defined by (3.23).

Substituting the corresponding values of the constants appearing in the expression (6.5), we check that no term vanishes if the corresponding values of integers $l_{(\frac{1}{2}p)}$, $\tilde{l}_{(\frac{1}{2}q)}$ satisfy $l_{(\frac{1}{2}p)} - \tilde{l}_{(\frac{1}{2}q)} - 2n = L + q$ except in the case $\tilde{l}_s = 1$, $l_{(\frac{1}{2}p)} = L + q + 1 + 2n$, where q are even. In that case $BY^{L,L+q+1+2n,1}$ has no components in $\mathfrak{H}^L_{L+q+2n,0}(H^p_q)$ and $\mathfrak{H}^L_{L+q+2+2n,0}(H^p_q)$, but this does not mean that the representation is reducible on $\mathfrak{H}^L(H^p_q)$ as B is skew-symmetric on $\mathfrak{L}$, and $BY^{L,L+q+2+2n,0}$ and $BY^{L,L+q+2n,0}$ have nonvanishing components in $\mathfrak{H}^L_{L+q+1+2n,1}(H^p_q)$.

The proof of the irreducibility of the representation $D^L(H^q_p)$ on the Hilbert space $\mathfrak{H}^L(H^q_p)$ is analogous.

(b) *The Case* $p \geq q = 2$

The proof of irreducibility of the representation $D^L(H^p_2)$ on the Hilbert space $\mathfrak{H}^L(H^p_2)$ is the same as in the previous case.

The representation of the group $SO(p, q)$ on the Hilbert space $\mathfrak{H}^L(H^2_p)$ reduces to two irreducible parts $D^L_\pm(H^2_p)$ on the subspaces

$$
\mathfrak{H}^L_\pm(H^2_p) = \sum \oplus \mathfrak{H}^L_{\pm|\tilde{m}_1|,l_{(p/2)}}(H^2_p),
$$

where the sum is taken over all nonnegative integers $|\tilde{m}_1|$, $l_{(\frac{1}{2}p)}$ such that $|\tilde{m}_1| - l_{(\frac{1}{2}p)} - 2n = L + p$, $n = 0, 1, 2, \cdots$. The proof of the irreducibility of both representations $D^L_\pm(H^2_p)$ on $\mathfrak{H}^L_\pm(H^2_p)$ is the same as in the previous case. The reducibility of the representation on the space $\mathfrak{H}^L(H^2_p) = \mathfrak{H}^L_+(H^2_p) \oplus \mathfrak{H}^L_-(H^2_p)$ can be easily understood from (4.6) and the fact that every operator B_{ij} (6.3) maps the subspace $\mathfrak{H}^L_{|(\tilde{m}_1)|,l_{(p/2)}}(H^2_p)$ only into those four subspaces $\mathfrak{H}^L_{|(\tilde{m}')|,l'_{(p/2)}}(H^2_p)$ for which $\tilde{m}'_1 - \tilde{m}_1 = \pm 1$, $l'_{(p/2)} - l_{(\frac{1}{2}p)} = \pm 1$. This follows from (6.1) and (6.5).

[20] M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1961).

(c) *The Case $q = 1$*

If $p > 2$, the structure of the Hilbert space $\mathfrak{K}^L(H_1^p)$ is

$$\mathfrak{K}^L(H_1^p) = \sum \oplus \mathfrak{K}^L_{l_{(p/2)}}(H_1^p), \tag{6.9}$$

where the sum is taken over all nonnegative integers $l_{(\frac{1}{2}p)} = L + 1, L + 2, \cdots$. The irreducibility is proved as in the previous case using the operator $B_{p,1}$ and the element (5.6)

$${}_{1,2}Y^{L,l_{(p/2)}}_{m_{(p/2)}}(\Omega) \equiv Y^{L,l_2,\cdots,l_{(p/2)}}_{m_1,\cdots,m_{(p/2)}}(\Omega),$$

where $m_2 = \cdots = m_{(\frac{1}{2}p)} = 0$ and $m_1, l_2, \cdots, l_{(\frac{1}{2}p)-1}$ have minimal possible values. The element $BY_0^{L,l_{(p/2)}}$ has non-vanishing components in

$$\mathfrak{K}^L_{l_{(p/2)}\pm 1}(H_1^p)$$

as is expressible in the form

$$(B_1 Y^{L,l})(\Omega) = -2A_+(l)\left[\frac{{}_2N(l+1)}{{}_1N(l)}\right]^{\frac{1}{2}} {}_1Z^{L,l+1}(\Omega) - 2A_-(l)\left[\frac{{}_2N(l-1)}{{}_1N(l)}\right]^{\frac{1}{2}} {}_1Z^{L,l-1}(\Omega), \tag{6.10}$$

$$(B_2 Y_0^{L,l})(\Omega) = -\tfrac{1}{2}(L+l+p-1)(L-l)A_+(l)\left[\frac{{}_1N(l+1)}{{}_2N(l)}\right]^{\frac{1}{2}} {}_2Z^{L,l+1}(\Omega)$$
$$-\tfrac{1}{2}(L-l+1)(L+l+p-2)A_-(l)\left[\frac{{}_1N(l-1)}{{}_2N(l)}\right]^{\frac{1}{2}} {}_2Z^{L,l-1}(\Omega), \tag{6.11}$$

where

$${}_{1,2}Z^{L,l}(\Omega) = \begin{cases} {}_{1,2}Y_0^{L,l}(\Omega), & \text{for } p \text{ odd}, \\ (2i)^{-1}[{}_{1,2}Y_1^{L,l}(\Omega) - {}_{1,2}Y_{-1}^{L,l}(\Omega)], & \text{for } p \text{ even}. \end{cases} \tag{6.12}$$

Here ${}_{1,2}N(l) = N_{(\frac{1}{2}p)} \cdot {}_{1,2}N$, where the constants $N_{(\frac{1}{2}p)}$ and ${}_{1,2}N$ are defined by the expressions (3.21) and (5.8). The nonvanishing feature of the coefficients can be checked as before.

If $p = 2$, there exist two irreducible representations $D^L_{\pm}(H_1^2)$ on the spaces

$$\mathfrak{K}^L_{\pm}(H_1^2) = \sum_{|m|=L+1}^{\infty} \oplus \mathfrak{K}^L_{\pm|m|}(H_1^2),$$

which can be proved as before.

B. Unitarity

The representation T_g of a group element $g \in SO(p, q)$ on the Hilbert space $\mathfrak{K}^L(H_q^p)$ is determined by the left-translation:

$$(T_g Y^{L,l_2,\cdots,l_{(p/2)},\tilde{l}_2,\cdots\tilde{l}_{(q/2)}}_{m_1,\cdots,m_{(p/2)},\tilde{m}_1,\cdots,\tilde{m}_{(q/2)}})(\Omega)$$
$$= Y^{L,l_2,\cdots,l_{(p/2)},\tilde{l}_2,\cdots\tilde{l}_{(q/2)}}_{m_1,\cdots,m_{(p/2)},\tilde{m}_1,\cdots,\tilde{m}_{(q/2)}}(g^{-1}\Omega) \tag{6.13}$$

then the representation of the corresponding Lie algebra given by (6.2) and (6.3). Here the symbol $g^{-1}\Omega$ represents the set of parameters $\varphi'^1, \cdots, \vartheta'^{(\frac{1}{2}q)}, \theta'$ of the point $\Omega' = g^{-1}\Omega$ on H_q^p, and

$$Y^{L,l_2,\cdots,l_{(p/2)},\tilde{l}_2,\cdots,\tilde{l}_{(q/2)}}_{m_1,\cdots,m_{(p/2)},\tilde{m}_1,\cdots,\tilde{m}_{(q/2)}}(\Omega)$$

is a harmonic function defined in the expressions (3.17), (4.7), or (5.6). Therefore, the unitarity follows from the left-invariance of the measure $d\mu(\Omega)$ on the corresponding hyperboloid H_q^p.

7. CONCLUSIONS

We devote this section to a brief review and discussion of the derived representations $D^L(H_q^p)$ of the group $SO(p, q)$.

A. The Case $p \geq q > 2$ (Sec. 3)

There exist two series of representations: $D^L(H_q^p)$ and $D^L(H_p^q)$, related respectively to hyperboloids H_q^p (3.1) and H_p^q (3.2). The nonnegative integers $l_{(\frac{1}{2}p)}$, $\tilde{l}_{(\frac{1}{2}q)}$, which determine respectively the irreducible representations of the subgroup $SO(p)$ and $SO(q)$ are not independent as in the case of continuous most degenerate representations, but are restricted by

$$l_{(\frac{1}{2}p)} - \tilde{l}_{(\frac{1}{2}q)} - 2n = L + q \quad \text{for} \quad H_q^p, \tag{7.1}$$

$$\tilde{l}_{(\frac{1}{2}q)} - l_{(\frac{1}{2}p)} - 2n = L + p \quad \text{for} \quad H_p^q, \tag{7.2}$$

where $l_{(\frac{1}{2}p)}$, $\tilde{l}_{(\frac{1}{2}q)}$, and n range through every such triplet of nonnegative integers which satisfy (7.1) and (7.2). These two conditions are respectively illustrated graphically in Fig. 2 and Fig. 3. Every node of the net in the figures represents a subspace $\mathfrak{K}^L_{l_{(p/2)},\tilde{l}_{(q/2)}}$ of an irreducible representation of the maximal compact subgroup $SO(p) \times SO(q)$ determined by a pair of integers $l_{(\frac{1}{2}p)}$ and $\tilde{l}_{(\frac{1}{2}q)}$. Generators L_{ij} of the compact type act inside the subspace $\mathfrak{K}^L_{l_{(p/2)},\tilde{l}_{(q/2)}}$. On the other hand, the generator

$B_{r,s}$ of the noncompact type maps the subspace $\mathfrak{K}^L_{l(p/s),l(q/s)}$ into four neighboring subspaces

$$\mathfrak{K}^L_{l+1,l+1},\ \mathfrak{K}^L_{l-1,l+1},\ \mathfrak{K}^L_{l+1,l-1},\ \mathfrak{K}^L_{l-1,l-1}$$

(graphically represented in Fig. 2).

All the representations $D^L(H^p_q)$ and $D^L(H^q_p)$ are unitarily inequivalent except for $p = q$, where we have only one series of representations $D^L(H^p_p)$.

B. The Case $p \geq q = 2$ (Sec. 4)

In general, there exist three series of representations. Before describing them, we wish to stress the fact that the irreducible representations of the subgroup $SO(2)$ are characterized by an integer $n\tilde{m}_1$, which also takes on negative values. Instead of the conditions (7.1) and (7.2), we have now

$$|l_{(\frac{1}{2}p)}| - |\tilde{m}_1| - 2n = L + 2 \quad \text{for} \quad H^p_2, \tag{7.3}$$

$$|\tilde{m}_1| - |l_{(\frac{1}{2}p)}| - 2n = L + p \quad \text{for} \quad H^2_p, \tag{7.4}$$

where $|l_{(\frac{1}{2}p)}|$, $|\tilde{m}_1|$, and n range through all such nonnegative integers so that (7.3) and (7.4) are satisfied. It follows from these conditions and conclusions of Sec. 4 that there exists only one series of representations, $D^L(H^p_2)$, related with the hyperboloid H^p_2, while there exist two series of representations $D^L_+(H^2_p)$ and $D^L_-(H^2_p)$ related with the hyperboloid H^2_p. Their graphical representations are given in Figs. 4, 5, and 6, respectively. The representations are unitarily inequivalent except for the case $p = q = 2$. In the latter case, two subgroups $SO(2)$ of the group $SO(2, 2)$ are indistinguishable, and we have

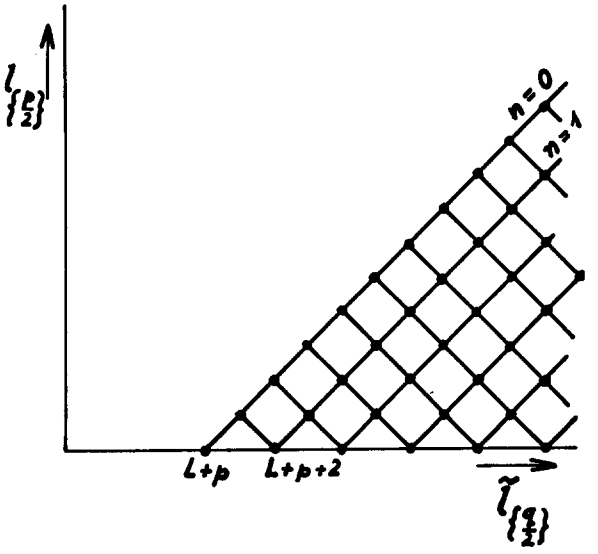

FIG. 3. Representation $D^L(H^q_p)$, $p \geq q > 2$.

only two unitarily inequivalent representations drawn in solid lines in Fig. 7. The representations appear after changing m_1 and $\tilde{m}_1$ are equivalent to a pair of previous representations. We represent them by dotted lines in Fig. 7.

C. The Case $q = 1$ (Sec. 4)

In general, there exists only one series of discrete most degenerate representations $D^L(H^p_1)$. However, in the case of $SO(2, 1)$, we have obtained two series of irreducible representations, i.e., $D^L_+(H^2_1)$ and

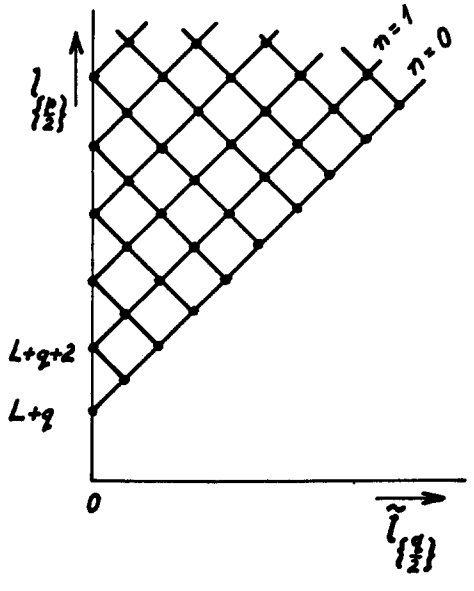

FIG. 2. Representation $D^L(H^p_q)$, $p \geq q > 2$.

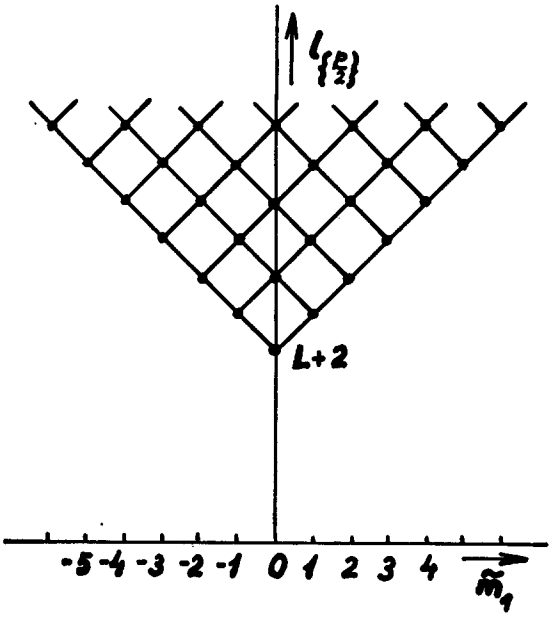

FIG. 4. Representation $D^L(H^p_2)$.

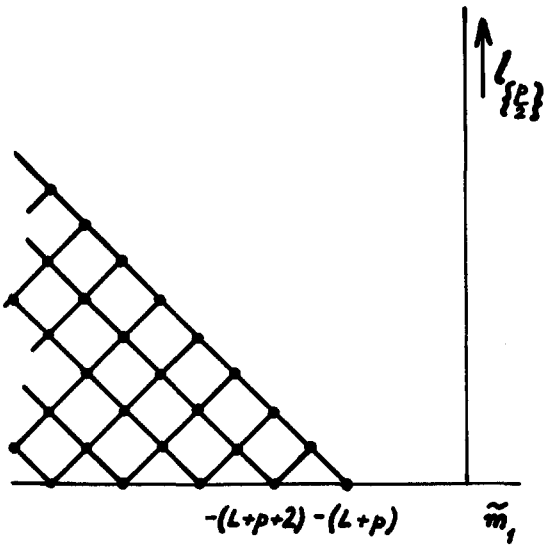

FIG. 5. Representation $D^L_-(H^2_p)$.

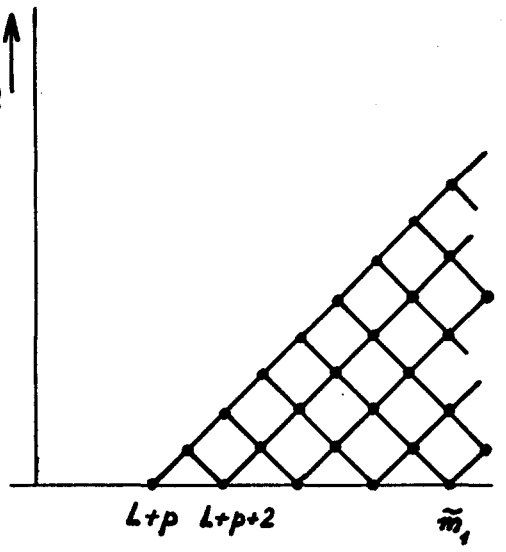

FIG. 6. Representation $D^L_+(H^2_p)$.

$D^L_-(H^2_1)$. The condition on the number $l_{(\frac{1}{2}p)}$, which determines the irreducible representations of the maximal compact subgroup $SO(p)$, has the form

$$|l_{(\frac{1}{2}p)}| = \max(L+1, 0) + n,$$
$$n = 0, 1, 2, \cdots . \tag{7.5}$$

It is interesting that we have found the discrete most degenerate representations even for the groups $SO(p, q)$ with odd p and q, which have no discrete nondegenerate principal series of representations (see Table I). Let us explain this unexpected fact, for example, for the Lorentz group $SO(3, 1)$. The action of two Casimir operators $\Delta_1 = \mathbf{M}^2 - \mathbf{N}^2$ and $\Delta_2 = \mathbf{M}\cdot\mathbf{N}$ on the basis f^k_r of the Hilbert space, which realizes the irreducible representation, can be written in the form[21]:

$$\Delta_1 f^k_r = -2(k_0^2 + c^2 - 1)f^k_r,$$
$$k_0 = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \cdots , \tag{7.6}$$
$$\Delta_2 f^k_r = -4ik_0 c f^k_r, \qquad c = i\rho, \quad \rho \in [0, \infty). \tag{7.7}$$

If we take the hyperboloid H^3_1 as the domain of the functions f^k_r, the second Casimir operator Δ_2 vanishes identically and the first operator admits discrete spectrum for $c = 0$:

$$\Delta_1 f^k_r = -2(k_0^2 - 1)f^k_r.$$

If we put $L = k_0 - 1$, the result agrees with that derived in Sec. 5.

For applications to physical problems with the $SO(p, q)$ symmetry, the derived discrete most degenerate representations $D^L(H^p_q)$ or $D^L(H^q_p)$ are especially convenient due to the facts that

i. The maximal set of the commuting operators is maximally reduced in these representations of $SO(p, q)$ groups. That is, for the discrete most degenerate representations of the $SO(p, q)$ group, the maximal set of commuting operators in the enveloping algebra consists of

$$\Delta[SO(p, q)],$$
$$C_p \equiv \begin{Bmatrix} \Delta[SO(p)], \Delta[SO(p-2)], \cdots , \Delta[SO(4)], & \text{for } p \text{ even} \\ \Delta[SO(p)], \Delta[SO(p-1)], \Delta[SO(p-3)], \cdots , \Delta[SO(4)], & \text{for } p \text{ odd} \end{Bmatrix},$$
$$\tilde{C}_q \equiv \begin{Bmatrix} \Delta[SO(q)], \Delta[SO(q-2)], \cdots , \Delta[SO(4)], & \text{for } q \text{ even} \\ \Delta[SO(q)], \Delta[SO(q-1)], \Delta[SO(q-3)], \cdots , \Delta[SO(4)], & \text{for } q \text{ odd} \end{Bmatrix}, \tag{7.8}$$
$$H \equiv \left\{ -\frac{\partial}{\partial\varphi^k}, -\frac{\partial}{\partial\bar{\varphi}^l}, \quad \begin{matrix} k = 1, 2, \cdots , [\frac{1}{2}p] \\ l = 1, 2, \cdots , [\frac{1}{2}q] \end{matrix} \right\},$$

[21] M. A. Naimark, *Linear Representations of the Lorentz Group* (Pergamon Press, Inc., New York, 1964), p. 167.

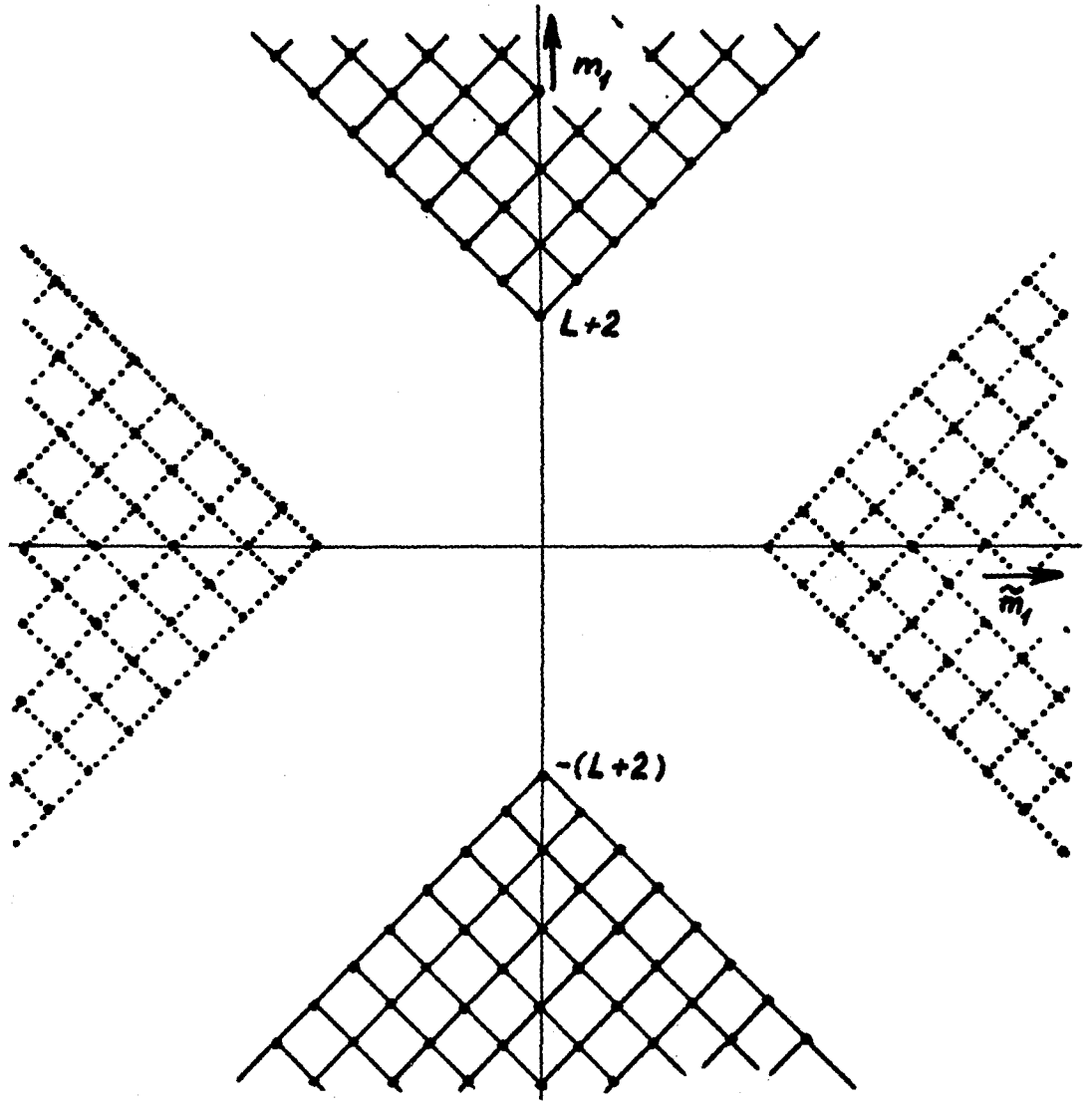

FIG. 7. Representation $D_{\omega}{}^{L}(H^{2}{}_{2})$.

where $\Delta[SO(p, q)]$ represents the Casimir operator of $SO(p, q)$, and C_p and $\tilde{C}_q$ the sequence of corresponding Casimir operators of the maximal compact subgroup $SO(p) \times SO(q)$. The set H contains operators of the Cartan subalgebra except when p and q are odd, in which case H represents the maximal Abelian compact subalgebra of $SO(p, q)$ (see Table I).

The number of operators contained in the maximal set of commuting operators in the enveloping algebra for the discrete most degenerate representations of $SO(p, q)$ is equal to

$$N = p + q - 1,$$

while the corresponding number for principal nondegenerate representations is

$$N' = \tfrac{1}{2}(r + l) = \tfrac{1}{4}[N(N + 1) + 2l],$$

where r and l are the dimension and the rank of $SO(p, q)$, respectively.

ii. The additive quantum numbers may be related to the eigenvalues of the set H. It turns out that the set H is largest in the biharmonic coordinate system, which we have used.

iii. The eigenfunctions of the maximal commuting set of operators are given in explicit form by formulas (3.17), (4.7), and (5.6); the range of the numbers $L_1 l_2, \cdots, l_{(\frac{1}{2}p)}, \tilde{l}_2, \cdots, \tilde{l}_{(\frac{1}{2}q)}, m_1, \cdots, m_{(\frac{1}{2}p)}, \tilde{m}_1, \cdots, \tilde{m}_{(\frac{1}{2}q)}$, which may play the role of quantum numbers, is determined by (3.20), (3.24), (4.9), and (5.9).

ACKNOWLEDGMENTS

The authors are indebted to Professor Abdu-Salam for his hospitality, and for valuable discussions. It is also a pleasure to thank Professor P.

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APPENDIX
THE MOST DEGENERATE REPRESENTATIONS OF THE COMPACT ROTATION GROUP $SO(p)$

The most degenerate representations of the compact rotation group $SO(p)$ were derived in Refs. 15 and 22. In this Appendix, we briefly review the main results, and we prove the irreducibility and unitarity of these representations.

For an arbitrary compact rotation group $SO(p)$, there exist the most degenerate representations on the finite-dimensional Hilbert space $\mathcal{H}(X)$ of functions, the domain X of which is the following Cartan symmetric space of rank one[9]

$$X^{p-1} = SO(p)/SO(p-1). \tag{A1}$$

The model of this space is a $(p-1)$-dimensional sphere S^{p-1}

$$(x^1)^2 + \cdots + (x^p)^2 = 1, \tag{A2}$$

imbedded in p-dimensional Euclidean space E^p.

Introducing the biharmonic coordinate system on the sphere S^{p-1} by formula (3.6) or (3.7), we can calculate the metric tensor $g_{\alpha\beta}(S^{p-1})$ on the sphere S^{p-1}, and, for the Laplace–Beltrami operator $\Delta(S^{p-1})$ defined by (2.1), we then obtain

$$\Delta(S^{2r-1}) = (\cos^2\vartheta^r)^{-1}\frac{\partial^2}{(\partial\varphi^r)^2} + (\sin^{2r-2}\vartheta^r\cos\vartheta^r)^{-1}\frac{\partial}{\partial\vartheta^r}(\sin^{2r-2}\vartheta^r\cos\vartheta^r)\frac{\partial}{\partial\vartheta^r} + \frac{\Delta(S^{2r-3})}{\sin^2\vartheta^r} \quad \text{for} \quad p = 2r, \quad r = 2, \cdots \tag{A3}$$

and $\Delta(S^1) = \partial^2/(\partial\varphi^1)^2$

$$\Delta(S^{2r}) = (\sin^{2r-1}\vartheta^{r+1})^{-1}\frac{\partial}{\partial\vartheta^{r+1}}(\sin^{2r-1}\vartheta^{r+1})\frac{\partial}{\partial\vartheta^{r+1}} + \frac{\Delta(S^{2r-1})}{\sin^2\vartheta^{r+1}} \quad \text{for} \quad p = 2r+1, \; r = 1, 2, \cdots, \tag{A4}$$

where $\Delta(S^{2r-3})$ and $\Delta(S^{2r-1})$ are again invariant operators of $SO(2r-2)$ and $SO(2r)$, respectively. Using induction, both operators $\Delta(S^{2r-3})$ and $\Delta(S^{2r-1})$ can be decomposed in the same way as $\Delta(S^{p-1})$ in (A3). The eigenvalues $\lambda_{(l_p)}$ of the Laplace–Beltrami operator on the sphere S^{p-1} are of the very well-known form

$$\lambda_{(l_p)} = -l_{(l_p)}(l_{(l_p)} + p - 2). \tag{A5}$$

Due to the inductive construction of the Laplace–Beltrami operators, we can separate variables in the eigenvalue problem for the operator $\Delta(S^{p-1})$. Thus, we obtain the differential equations:

$$\left[\frac{1}{\sin^{(2r-3)}\vartheta^r\cos\vartheta^r}\frac{\partial}{\partial\vartheta^r}\sin^{(2r-3)}\vartheta^r\cos\vartheta^r\frac{\partial}{\partial\vartheta^r} - \frac{m_r^2}{\cos^2\vartheta^r} - \frac{l_{r-1}(l_{r-1}+2r-4)}{\sin^2\vartheta^r} + l_r(l_r+2r-2)\right]\psi^{l_r}_{m_r,l_{r-1}}(\vartheta^r) = 0 \quad \text{if} \quad p = 2r \tag{A6}$$

and

$$\left[\frac{1}{\sin^{(2r-1)}\vartheta^{r+1}}\frac{\partial}{\partial\vartheta^{r+1}}\sin^{(2r-1)}\vartheta^{r+1}\frac{\partial}{\partial\vartheta^{r+1}} - \frac{l_r(l_r+2r-2)}{\sin^2\vartheta^{r+1}} + l_{r+1}(l_{r+1}+2r-1)\right]\cdot\psi^{l_{r+1}}_{l_r}(\vartheta^{r+1}) = 0, \quad \text{if} \quad p = 2r+1. \tag{A7}$$

Solutions of the equations (A6) or (A7) belonging to the Hilbert space of square integrable functions with respect to the measure

$$d\mu(\omega) = [\bar{g}(S^{p-1})]^{\frac{1}{2}}\,d\omega = \begin{cases} \prod_{k=2}^{r}\cos(\vartheta^k)\cdot\sin^{(2k-3)}(\vartheta^k)\cdot d\vartheta^k\cdot\prod_{k=1}^{r}d\varphi^k & \text{for} \quad p = 2r, \\ \sin^{2r-1}(\vartheta^{r+1})\,d\vartheta^{r+1}\prod_{k=2}^{r}\cos(\vartheta^k)\cdot\sin^{(2k-3)}(\vartheta^k)\cdot d\vartheta^k\cdot\prod_{k=1}^{r}d\varphi^k & \text{for} \quad p = 2r+1, \end{cases} \tag{A8}$$

are given as follows:

[22] N. Ya. Vilenkin, Tr. Mosk. Mat. Obshch. 12, 185, (1963).

For $p = 2r$, $r = 2, \cdots$

$$\psi^{l_r}_{m_r,l_{r-1}}(\vartheta^r) = \tan^{|l_{r-1}|}\vartheta^r \cos^{l_r}\vartheta^r \cdot {}_2F_1[\tfrac{1}{2}(|l_{r-1}| - l_r + m_r), \tfrac{1}{2}(|l_{r-1}| - l_r - m_r); l_{r-1} + r - 1; -\tan^2\vartheta^r], \tag{A9}$$

for $p = 2$

$$\psi_{m_1}(\varphi^1) = (2\pi)^{-\frac{1}{2}} \cdot \exp im_1\varphi^1,$$

where l_r, l_{r-1}, and m_r are restricted by the condition of square-integrability of solutions of (A3), i.e.,

$$-l_r + |l_{r-1}| + |m_r| = -2n,$$
$$n = 0, 1, \cdots, [\tfrac{1}{2}l_r] \tag{A10}$$

and for $p = 2r + 1$, $r = 1, 2, \cdots$

$$\psi^{l_{r+1}}_{l_r}(\vartheta^{r+1}) = \tan^{l_r}\vartheta^{r+1} \cdot \cos^{l_{r+1}}\theta^{r+1} \cdot {}_2F_1[\tfrac{1}{2}(l_r - l_{r+1}); \tfrac{1}{2}(l_r - l_{r+1} + 1); l_r + r; -\tan^2\vartheta^{r+1}] \tag{A11}$$

with the restriction

$$l_r - l_{r+1} = -n \qquad n = 0, 1, \cdots, l_{r+1}. \tag{A12}$$

Both solutions (A9) and (A11) can be expressed in terms of d-functions[20] and exponential functions. The basis of the Hilbert space $\mathfrak{H}^{l_r}(S^{p-1})[\mathfrak{H}^{l_{r+1}}(S^{p-1})]$ is then given by expressions in (3.18).

A. Irreducibility

(A) $p = 2r$, $r = 1, 2, \cdots$. The proof is based on induction. The representation $D^{m_1}(S^1)$ of the group $SO(2)$ is irreducible on the one-dimensional space $\mathfrak{H}^{m_1}(S^1)$ determined by the vector

$$Y_{m_1}(\varphi^1) = (2\pi)^{-\frac{1}{2}} \exp(im_1\varphi^1).$$

Let us suppose that the representation $D^{l_{r-1}}(S^{p-3})$ is irreducible on $\mathfrak{H}^{l_{r-1}}(S^{p-3})$, and then let us show that the representation $D^{l_r}(S^{p-1})$ must be irreducible on $\mathfrak{H}^{l_r}(S^{p-1})$. Denoting $\mathfrak{H}^{l_r}_{l_{r-1},m_r} = \mathfrak{H}^{l_{r-1}}(S^{p-3}) \otimes \mathfrak{H}^{m_r}(S^1)$, we can represent the space $\mathfrak{H}^{l_r}(S^{p-1})$ in the form

$$\mathfrak{H}^{l_r}(S^{p-1}) = \sum \oplus\, \mathfrak{H}^{l_r}_{l_{r-1},m_r}, \tag{A13}$$

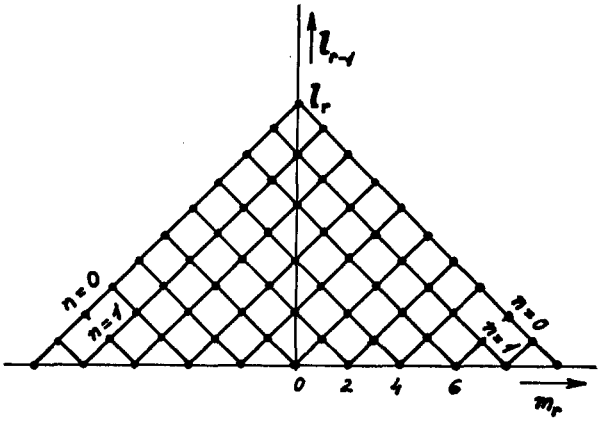

FIG. 8. Representation $D^{l_r}(S^{2r-1})$.

where the sum is taken over all such integers l_{r-1}, m_r, which satisfy the condition $|l_{r-1}| + |m_r| + 2n = l_r$, $n = 0, 1, 2, \cdots, [\tfrac{1}{2}l_r]$. (In the following we use the convention $l_{r-1} = m_1$ for $r = 2$.) The decomposition (A13) is represented by the net in Fig. 8, where the nodes correspond to the subspaces $\mathfrak{H}^{l_r}_{l_{r-1},m_r}$. Hence, to prove the irreducibility of the representation $D^{l_r}(S^{p-1})$, it is sufficient to show that the vector $(L_{r-1,r-2}\phi^{l_r,l_{r-1}}_{m_r,0})(\omega)$ has nonvanishing components in all four possible neighboring subspaces $\mathfrak{H}^{l_r}_{l_{r-1}\pm1,m_r\pm1}$. Here $L_{r-1,r-2}$ is defined by (6.2) and

$$\phi^{l_r,l_{r-1}}_{m_r,m_{r-1}}(\omega) = \psi^{l_r}_{m_r,l_{r-1}}(\vartheta^r) \cdot Y^{l_2,\cdots,l_{r-1}}_{m_1,\cdots,m_{r-1}}(\varphi^1, \vartheta^2, \cdots, \vartheta^{r-1}) \times (2\pi)^{-\frac{1}{2}} \cdot \exp im_r\varphi^r.$$

$$\begin{aligned}
&(L_{r-1,r-2}\phi^{l_r,l_{r-1}}_{m_r,0})(\omega) \\
&= \frac{(l_{r-1} + m_r - l_r)(l_{r-1} + m_r + l_r + p - 2)}{2l_{r-1} + p - 2} A_+(l_{r-1})A_+(m_r)\left[\frac{N(l_{r-1}+1)}{N(l_{r-1})}\right]^{\frac{1}{2}} Z^{l_r,l_{r-1}+1}_{m_r+1}(\omega) \\
&+ (2l_{r-1} + p - 4) \cdot A_-(l_{r-1})A_+(m_r)\left[\frac{N(l_{r-1}-1)}{N(l_{r-1})}\right]^{\frac{1}{2}} Z^{l_r,l_{r-1}-1}_{m_r+1}(\omega) \\
&+ \frac{(l_{r-1} - m_r - l_r)(l_{r-1} - m_r + l_r + p - 2)}{2l_{r-1} + p - 2} \cdot A_+(l_{r-1})A_-(m_r)\left[\frac{N(l_{r-1}+1)}{N(l_{r-1})}\right]^{\frac{1}{2}} Z^{l_r,l_{r-1}+1}_{m_r-1}(\omega) \\
&+ (2l_{r-1} + p - 4) \cdot A_-(l_{r-1})A_-(m_r)\left[\frac{N(l_{r-1}-1)}{N(l_{r-1})}\right]^{\frac{1}{2}} Z^{l_r,l_{r-1}-1}_{m_r-1}(\omega),
\end{aligned} \tag{A14}$$

where

$$Z^{l_r,l_{r-1}}_{m_r}(\omega) = (2i)^{-1}\phi^{l_r,l_{r-1}}_{m_r,+1}(\omega) - (2i)^{-1}\phi^{l_r,l_{r-1}}_{m_r,-1}(\omega).$$

The coefficients $A_\pm(l_{r-1})$ are defined by the expression (6.7), $A_\pm(m_r) = (2i)^{-1}$, and $N(l_{r-1}) = N_{r-1}$ is defined by (3.21).

The coefficients in the expression (A14) do not vanish for any two nonnegative integers l_{r-1}, m_r satisfying the condition $|l_{r-1}| + |m_r| + 2n = l_r$, $n = 0, 1, \cdots, [\frac{1}{2}l_r]$, except $A_-(l_{r-2})$ for $l_{r-1} = 1$. However, the mapping

$$\mathcal{H}^{l_r}_{1,m_r} \xrightarrow{L_{r-1,r-2}} \mathcal{H}^{l_r}_{0,m_r\pm1}$$

is possible as the operator $L_{r-1,r-2}$ is skew-symmetric on $\mathcal{H}^{l_r}(S^{p-1})$ and $(L_{r-1,r-2}\phi^{l_r,0}_{m_r\pm1,0}, Z^{l_r,1}_{m_r}) \neq 0$, where $\phi^{l_r,0}_{m_r\pm1,0} \in \mathcal{H}^{l_r}_{0,m_r\pm1}$ and $Z^{l_r,1}_{m_r} \in \mathcal{H}^{l_r}_{1,m_r}$.

(B) $p = 2r + 1$, $r = 1, 2, \cdots$. Using the operator $L_{r+1,r}$ and the element

$$\phi^{l_r,l_{r-1}}(\omega) = \psi^{l_r}_{0,l_{r-1}}(\vartheta^r)\, Y^{l_2,\cdots,l_{r-1}}_{0,0,\cdots,0}(\varphi^1, \vartheta^2, \cdots, \varphi^{r-1}, \vartheta^{r-1}),$$

where $l_2, \cdots, l_{r-1}$ take the minimal possible values, we prove the irreducibility of the representation $D^{l_r+1}(S^{p-1})$ on the space $\mathcal{H}^{l_r+1}(S^{p-1})$ from the irreducibility of the representations $D^{l_r}(S^{p-2})$ on $\mathcal{H}^{l_r}(S^{p-3})$ as before. The irreducibility of the representations $D^{l_r}(S^{p-2})$ on $\mathcal{H}^{l_r}(S^{p-2})$ have been proved in the previous case.

B. Unitarity

Due to the left-invariance of the measure $d\mu(\omega)$ (A8) on the sphere S^{p-1}, the representations $D^{l_r}(S^{p-1})$ and $D^{l_r+1}(S^{p-1})$ are unitary.

The Momentum Autocorrelation Function in a Bernoulli Chain

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This paper is devoted to the study of the statistical dynamics of the small amplitude coplanar vibrations of a compound pendulum consisting of $N + 1$ particles suspended in series by weightless strings in a gravitational field. All particles have the same mass m, except for the top particle whose mass is $m(1 + \mathcal{Q})$; and all strings are of equal length. The behavior of this system in the limit in which $N \to \infty$ is of particular interest, because the maximum normal mode frequency is proportional to $N^{1/2}$. In the limit $N \to \infty$, asymptotic formulas with error estimates are obtained for the time dependence of the momentum autocorrelation function of: (1) the top particle when $\mathcal{Q} = 0$; (2) the bottom particle when $\mathcal{Q} = 0$; and (3) the top particle when $N \gg \mathcal{Q} \gg 1$.

A. INTRODUCTION

RECENTLY a large number of investigations of the statistical dynamical behavior of systems of coupled harmonic oscillators have appeared in the literature.[1-18] The object of this work has been to gain insight into the properties of time-relaxed correlations between small numbers of oscillator variables. Only three investigations[1,3,5] have dealt explicitly with the dependence of correlations on the number of oscillators N as N approaches infinity; and all three were concerned with the same system, a one-dimensional model of a crystal with nearest-neighbor interactions and periodic boundary conditions. The purpose of this paper is to study a different one-dimensional oscillator model with nearest-neighbor interactions in which there is an essential dependence of the momentum autocorrelation on N. Our model, first considered by D. Bernoulli,[19] deals with the small amplitude coplanar vibrations of a compound pendulum consisting of a large number of particles suspended in series in a gravity field by means of weightless connecting strings. Figure 1 is a reproduction of the figures in the Bernoulli paper of 1732 showing the 2-, 3-, and ∞-particle chains. The restoring force on a displaced particle in a Bernoulli chain is roughly proportional to the number of particles suspended below it. Consequently, there is a significant difference between the dynamical behavior of a particle near the top of the chain and that near the bottom of the chain. Furthermore, the maximum normal mode frequency of the chain is proportional to the square root of the number of particles in the system. These properties are in marked contrast to those of the one-dimensional crystal model[5] in which all particles are dynamically equivalent, and in which the maximum normal mode frequency approaches a constant as the number of particles in the crystal is increased.

In the remainder of this section, we outline the calculations contained in the paper. They are based on the following solution to the general problem of

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[19] D. Bernoulli, Commentarii Academiae Scientiarum Imperialis Petropolitanae **6**, 108 (1732); **7**, 162 (1734). [This journal is cataloged under "Akad. Nauk SSSR, Leningrad" in *Union List of Serials*, W. Gregory, Ed. (W. H. Wilcox Company, New York, 1943), 2nd ed.] These papers contain a treatment of the oscillations of a double and a triple pendulum, a figure depicting a five-particle pendulum, and the classic treatment of the continuum limit in which the Bessel function $J_0(x)$ occurs.

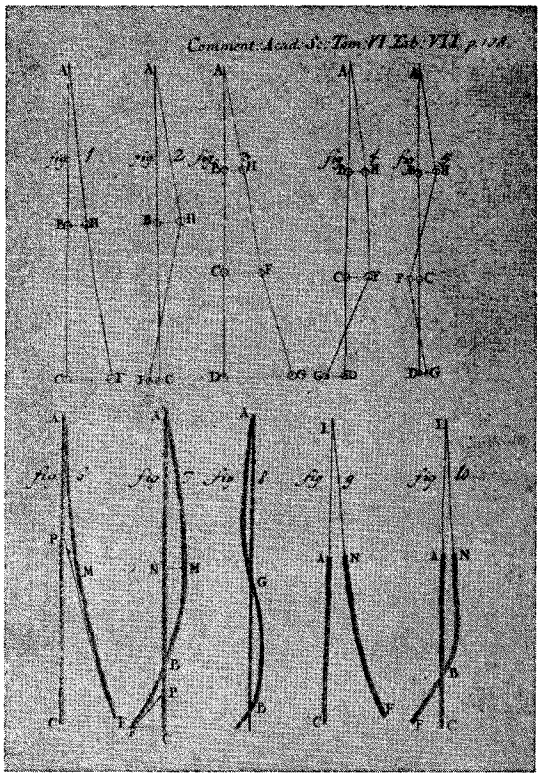

FIG. 1. Reproduction of the figures in the Bernoulli paper of 1732 showing configurations of the 2- and 3-particle chains and of the continuum limit of the chain.

calculating the normalized momentum autocorrelation function of a particle in a coupled oscillator system[5,6]

$$\rho_n(t) = \sum_{\nu=1}^{N} X_{n\nu}^2 \cos s_\nu t, \qquad (1)$$

where $\rho_n(t)$ is the normalized momentum autocorrelation function of a particle n in a classical system in a canonical distribution at temperature T,

$$\rho_n(t) = \langle P_n(t')P_n(t' + t)\rangle / \langle P_n^2(t')\rangle.$$

The coefficient $X_{n\nu}$ is the amplitude of particle n in the νth normalized normal mode vector, and s_ν is frequency of the νth normal mode. Thus, the calculation of $\rho_n(t)$ requires a knowledge of the normal mode eigenfrequencies and eigenvectors. Our model is a Bernoulli chain consisting of $N + 1$ particles numbered from $n = 0$ to $n = N$ starting at the bottom particle. The lengths of all connecting strings are equal to l; and the masses of all particles are equal to m except for the topmost particle $n = N$ whose mass is $m(1 + \mathcal{Q})$. In Sec. B, we calculate the values of $X_{n\nu}$ and s_ν. The values of $X_{n\nu}$ and s_ν for the case in which the top mass is equal to the others have been obtained by Bottema.[20] We have merely modified his calculation to account for the change in the mass of particle N. In Sec. C, we estimate the time dependence of the momentum autocorrelation in three particular cases and obtain rigorous bounds on the errors in the estimates. The three cases treated are: (1) $\rho_N(t)$ when $\mathcal{Q} = 0$, (2) $\rho_0(t)$ when $\mathcal{Q} = 0$, and (3) $\rho_N(t)$ when $N \gg \mathcal{Q} \gg 1$. The exact formula for the momentum autocorrelation function of a particle in a Bernoulli chain of $N + 1$ identical particles ($\mathcal{Q} = 0$) is obtained immediately by substituting in Eq. (1) the values of $X_{n\nu}$ and s_ν obtained by Bottema. The result can be written as

$$\rho_n = \frac{1}{N+1} \sum_{\nu=1}^{N+1} \frac{k_\nu}{N+1} \left(\frac{L_n(k_\nu)}{L_N(k_\nu)}\right)^2 \cos\left[(k_\nu l/g)^{\frac{1}{2}} t\right], \qquad (2)$$

where $L_n(x)$ is the Laguerre polynomial of order N, the numbers k_ν, $\nu = 1, \cdots, N + 1$, are the zeros of $L_{N+1}(x)$, and g is the gravitational constant. The estimates which are obtained in Sec. C for $\rho_0(t)$ and $\rho_N(t)$ are based on three observations. First, the sum of the coefficients of the cosine in Eq. (2) is identically equal to unity. Second, when the number N is large compared to unity, there is an asymptotic series[21] for $L_N(x)$ which is uniformly valid in the oscillatory range $0 < x < 4N + 2$ and which provides accurate values for k_ν and $[L_N(k_\nu)]^{-2}$. Third, when the asymptotic formulas are substituted in Eq. (2), the resulting sum is obviously related to an integral. There is a simple upper bound on the magnitude of the difference between the sum and the approximating integral which involves the number of terms in the sum and the total variation of the integrand.

Finally, in Sec. D, we discuss some of the results obtained for the Bernoulli chain; and we relate these results to those obtained in other models. A comparison of $\rho_0(t)$ and $\rho_N(t)$ when $\mathcal{Q} = 0$ shows two extremes in the behavior of the momentum autocorrelation function. In the case of $\rho_N(t)$, when $\mathcal{Q} = 0$ and $N \gg \mathcal{Q} \gg 1$, there is a significant dependence on the number of particles in the chain. The difference between the results in the last two cases illustrates the inhibiting effect of a large mass difference on the rate of transfer of momentum in harmonic oscillator models. This inhibiting effect is of considerable interest and has been studied in simple crystal models where various correlation functions of a heavy particle have been shown to

[20] O. Bottema, Jahresber. Deut. Math.-Verein. **42**, 42 (1933).

[21] F. G. Tricomi, *Differential Equations* (Hafner Publishing Company, New York, 1961), p. 190.

exhibit classic Brownian-like properties in the case of one-[2,3,6,7] and three-dimensional[9] crystals.

B. NORMAL MODE EIGENFREQUENCIES AND EIGENVECTORS IN A BERNOULLI CHAIN

Consider a Bernoulli chain, or compound pendulum, consisting of $N+1$ particles at equal distances l along a string suspended in a gravity field. The mass of the connecting string is neglected and we are only concerned with small transverse coplanar oscillations of the particles. The particles, numbered from 0 to N starting at the bottom, have the same mass m with the exception of the top particle which has the mass $(1+\mathcal{Q})m$. The tension S_i in the string between the ith and $(i-1)$th particle is given by

$$S_i = img, \qquad i = 1, \cdots, N, \tag{3}$$

where g is the gravitational constant; and the tension S_{N+1} in the string connecting the uppermost particle to the suspension point is given by

$$S_{N+1} = (N + \mathcal{Q} + 1)mg.$$

If we denote the transverse displacement of the particles from their equilibrium positions by x_i, then the net force on particle i is

$$S_{i+1}(x_{i+1} - x_i)/l - S_i(x_i - x_{i-1})/l.$$

The Hamiltonian for small amplitude vibrations of the system is

$$H = \sum_{i=0}^{N-1} \frac{p_i^2}{2m} + \frac{p_N^2}{2m(1+\mathcal{Q})} + \sum_{i=0}^{N-1} \frac{S_{i+1}}{2l}(x_{i+1} - x_i)^2 + \frac{S_{N+1}}{2l} x_N^2, \tag{4}$$

where p_i is the momentum conjugate to x_i. We transform the Hamiltonian to diagonal form by following the procedure used by Bottema[20] in the case in which all masses are equal, $\mathcal{Q} = 0$. First apply the following canonical transformation in (4)

$$p_i = m^{\frac{1}{2}}P_i, \qquad x_i = m^{-\frac{1}{2}}Q_i, \qquad i = 0, 1, \cdots, N-1, \tag{5}$$

$$p_N = (1+\mathcal{Q})^{\frac{1}{2}}m^{\frac{1}{2}}P_N, \qquad x_N = (1+\mathcal{Q})^{-\frac{1}{2}}m^{-\frac{1}{2}}Q_N.$$

This yields for the Hamiltonian

$$H = \sum_{i=0}^{N} \tfrac{1}{2}P_i^2 + \sum_{i=0}^{N-2} \tfrac{1}{2}\omega_0^2(i+1)(Q_{i+1} - Q_i)^2 + \tfrac{1}{2}\omega_0^2 N[Q_N/(1+\mathcal{Q})^{\frac{1}{2}} - Q_{N-1}]^2 + \tfrac{1}{2}\omega_0^2(N + \mathcal{Q} + 1)(\mathcal{Q}+1)^{-1}Q_N^2, \tag{6}$$

where

$$\omega_0^2 = gl^{-1}. \tag{7}$$

To diagonalize the Hamiltonian (6), we construct an orthonormal transformation which diagonalizes the potential energy. The equations of the associated eigenvalue problem are

$$\begin{aligned} &-iQ_{i-1} + (2i + 1 - k)Q_i - (i+1)Q_{i+1} = 0, \qquad i = 0, \cdots, N-2, \\ &-(N-1)Q_{N-2} + (2N - 1 - k)Q_{N-1} - N(1+\mathcal{Q})^{-\frac{1}{2}}Q_N = 0, \\ &-N(1+\mathcal{Q})^{-\frac{1}{2}}Q_{N-1} + [2N(1+\mathcal{Q})^{-1} + 1 - k]Q_N = 0. \end{aligned} \tag{8}$$

In (8) the first $N-1$ equations have the form of the recurrence relations of the Laguerre polynomials, $L_N(k)$, so that we may put

$$Q_i(k) = L_i(k), \qquad i = 0, \cdots, N-2. \tag{9}$$

Then we deduce from the Nth equation

$$Q_N(k) = (1+\mathcal{Q})^{\frac{1}{2}}L_N(k); \tag{10}$$

and consequently the last equation gives the eigenvalues k_ν,

$$NL_{N-1}(k) - [2N + (1+\mathcal{Q})(1-k)]L_N(k) = 0. \tag{11}$$

Applying the recurrence relation between $L_{N-1}(k)$, $L_N(k)$, and $L_{N+1}(k)$, the eigenvalue equation can also be written as

$$(N+1)L_{N+1}(k) + \mathcal{Q}(1-k)L_N(k) = 0. \tag{12}$$

Clearly this equation has $N+1$ roots k_ν which are separated by the zeros of $L_N(k)$. Thus, the components of the eigenvectors of the equations are

$$L_i(k_\nu), \qquad i = 0, \cdots, N-1; \nu = 1, \cdots, N+1, \tag{13}$$

and

$$(1+\mathcal{Q})^{\frac{1}{2}}L_N(k_\nu).$$

To normalize the eigenvectors we use the property[22]

$$\sum_{i=0}^{N} (L_i(k))^2 = (N+1)\left[L_{N+1}(k)\frac{d}{dk}L_N(k) - L_N(k)\frac{d}{dk}L_{N+1}(k)\right]. \tag{14}$$

Combining the recurrence Eq. (8) with (12) and the relations[22]

$$k(d/dk)L_N(k) = N[L_N(k) - L_{N-1}(k)], \tag{15}$$

[22] G. Szegö, *Orthogonal Polynomials* (American Mathematical Society, New York, 1939), Chap. 5.

and

$$(d/dk)L_{N+1}(k) = (d/dk)L_N(k) - L_N(k), \qquad (16)$$

we obtain for the components $X_{i\nu}$ of the normalized eigenvectors in Eq. (11)

$$X_{i\nu} = k_\nu^{\frac{1}{2}}[\mathcal{Q}(1+\mathcal{Q})k_\nu^2 - 2\mathcal{Q}k_\nu(N+\mathcal{Q}+1) + (N+\mathcal{Q}+1)^2]^{-\frac{1}{4}}L_i(k_\nu)/L_N(k_\nu), \quad i = 0, \cdots, N-1 \qquad (17)$$

and

$$X_{N\nu} = (1+\mathcal{Q})^{\frac{1}{4}}k_\nu^{\frac{1}{2}}[\mathcal{Q}(1+\mathcal{Q})k_\nu^2 - 2\mathcal{Q}k_\nu(N+\mathcal{Q}+1) + (N+\mathcal{Q}+1)^2]^{-\frac{1}{4}}.$$

Now the transformed Hamiltonian is written

$$H = \sum_{\nu=1}^{N+1} \tfrac{1}{2}(\mathfrak{p}_\nu^2 + s_\nu^2 q_\nu^2), \qquad s_\nu^2 = \omega_0^2 k_\nu^2, \qquad (18)$$

where

$$\mathfrak{p}_\nu = \sum_{i=0}^{N} X_{i\nu}P_\nu, \qquad q_\nu = \sum_{i=0}^{N} X_{i\nu}Q_\nu.$$

The values of $X_{i\nu}^2$ and s_ν^2 in Eqs. (17) and (18) reduce to the values obtained by Bottema for $\mathcal{Q} = 0$,

$$X_{i\nu}^2 = (N+1)^{-2}k_\nu[L_i(k_\nu)/L_N(k_\nu)]^2 \qquad (19)$$

and

$$s_\nu^2 = \omega_0^2 k_\nu, \qquad \nu = 1, \cdots, N+1$$

where k_ν is the νth zero of $L_{N+1}(k)$.

C. EXPLICIT TIME DEPENDENCE OF THE MOMENTUM AUTOCORRELATION FUNCTION

The explicit time dependence of the momentum autocorrelation function will be determined in three particular cases (1) $\rho_N(t)$ when $\mathcal{Q} = 0$, (2) $\rho_0(t)$ when $\mathcal{Q} = 0$, and (3) $\rho_N(t)$ when $1 \ll \mathcal{Q} \ll N$. In each case, the procedure is based on the three observations listed in Sec. A.

1. $\rho_N(t)$ When $\mathcal{Q} = 0$

The expression for $\rho_N(t)$ when $\mathcal{Q} = 0$ follows from Eq. (2) and can be written as

$$\rho_N(t) = \frac{4}{N+1}[1 + \tfrac{1}{2}(N+1)^{-1}] \sum_{\nu=1}^{N+1} \frac{k_\nu}{4N+6} \times \cos\left[\omega_0\left(\frac{k_\nu}{4N+6}\right)^{\frac{1}{2}}(4N+6)^{\frac{1}{2}}t\right], \qquad (20)$$

where $\omega_0^2 = g/l$, and k_ν is the νth zero of $L_{N+1}(k)$. In the limit $N \gg 1$, the $N+1$ zeros of $L_{N+1}(k)$, when normalized to $4N+6$, fill the interval $(0, 1)$. In this limit the k_ν's can be expressed implicitly in terms of ν with the aid of the following asymptotic formula for Laguerre polynomials of large order[21]:

$$\exp(-\tfrac{1}{2}k)L_{N+1}(k) \sim (-1)^{N+1}[\pi(N+\tfrac{3}{2})\sin 2\theta]^{-\frac{1}{2}} \times \sin[(N+\tfrac{3}{2})(2\theta - \sin 2\theta) + \tfrac{1}{4}\pi], \qquad (21)$$

where $\theta = \cos^{-1}[k/(4N+6)]^{\frac{1}{2}}$. The asymptotic formula is valid in the interval $\epsilon \leq k/(4N+6) \leq 1$, where ϵ is a fixed positive number, and the correction term is proportional to $N^{-\frac{1}{2}}$. The zeros of $L_{N+1}(k)$ correspond to those values of θ for which the argument of the sine function in Eq. (21) is a multiple of π,

$$(N+\tfrac{3}{2})(2\theta_\nu - \sin 2\theta_\nu) + \tfrac{1}{4}\pi = (N+2-\nu)\pi, \quad \nu = 1, \cdots, N+1 \qquad (22)$$

or

$$1 - \frac{2}{\pi}\left[\cos^{-1}\left(\frac{k_\nu}{4N+6}\right)^{\frac{1}{2}} - \left(\frac{k_\nu}{4N+6}\right)^{\frac{1}{2}}\left(1 - \frac{k_\nu}{4N+6}\right)^{\frac{1}{2}}\right] = \frac{\nu - \frac{1}{4}}{N+1} - \frac{1}{2N+3}\left(\frac{\nu - \frac{1}{4}}{N+1}\right). \qquad (23)$$

Equation (23) relates ν to $k_\nu/(4N+6)$. In the limit $N \gg 1$, the last term on the right-hand side can be neglected. In order to estimate the time dependence of $\rho_N(t)$, we determine the integral for which the right-hand side of Eq. (20) is the discrete approximation. The integral in this case is

$$g(t) = \int_0^1 4w^2(\mu)\cos[w(\mu)\omega_0(4N+6)^{\frac{1}{2}}t]\,d\mu, \qquad (24)$$

where the sum is based on the points

$$\mu = \frac{\nu - \frac{1}{4}}{N+1}, \qquad \nu = 1, \cdots, N+1,$$

and where $w^2(\mu) = k_\nu/(4N+6)$ is related to μ by the limiting form of Eq. (23) for large N,

$$\mu = 1 - \frac{2}{\pi}[\cos^{-1}w(\mu) - w(\mu)[1 - w^2(\mu)]^{\frac{1}{2}}]. \qquad (25)$$

Thus, the discrete approximation for $g(t)$ is

$$\rho_N(t) \cong \frac{4}{N+1}\sum_{\nu=1}^{N+1} w^2\left(\frac{\nu - \frac{1}{4}}{N+1}\right) \times \cos\left[w\left(\frac{\nu - \frac{1}{4}}{N+1}\right)\omega_0(4N+6)^{\frac{1}{2}}t\right], \qquad (26)$$

where we have ignored the term $(1/2)(N+1)^{-1}$ in the coefficient of the sum in Eq. (20). The magnitude of the difference between the integral $g(t)$ in Eq. (24)

and the sum for $\rho_N(t)$ in Eq. (26) satisfies the following inequality[23]:

$$|g(t) - \rho_N(t)| \leq (N+1)^{-1}\mathcal{V}(N, t), \tag{27}$$

where $\mathcal{V}(N, t)$ is the variation of the integrand in the interval (0, 1). In the present case, where the derivative of the integrand in (20) is a continuous function of μ and $w(\mu)$ is an increasing function of μ, the variation $\mathcal{V}(N, t)$ is

$$\mathcal{V}(N, t) = \int_0^1 \left|\frac{d}{d\mu}\{4w^2(\mu)\cos[\omega_0 w(\mu)(4N+6)^{\frac{1}{2}}t]\}\right| d\mu$$

$$= 4\int_0^1 |2\cos[\omega_0 w(\mu)(4N+6)^{\frac{1}{2}}t] - w(\mu)\omega_0(4N+6)^{\frac{1}{2}}t\sin[\omega_0 w(\mu)(4N+6)^{\frac{1}{2}}t]|\, w(\mu)\frac{dw(\mu)}{d\mu}\, d\mu,$$

and satisfies the following inequality

$$\mathcal{V}(N, t) \leq 4\int_0^1 [2 + w(\mu)\omega_0(4N+6)^{\frac{1}{2}}t]w(\mu)\frac{dw(\mu)}{d\mu}d\mu$$

$$\leq 4[1 + \tfrac{1}{3}\omega_0 t(4N+6)^{\frac{1}{2}}]. \tag{28}$$

Combining Eqs. (28) and (27), and neglecting N^{-1} compared to unity, one obtains

$$|g(t) - \rho_N(t)| \leq 4N^{-1} + (8/3)\omega_0 t N^{-\frac{1}{2}}. \tag{29}$$

The initial value of $\rho_N(t)$ is unity. Therefore, it follows from Eq. (29) that the integral $g(t)$ is a useful approximation for $\rho_N(t)$ provided that $4N^{-1} + (8/3)\omega_0 t N^{-\frac{1}{2}}$ can be neglected when compared with $g(t)$.

The integral $g(t)$ in Eq. (24) is easily evaluated after changing the variable of integration from μ to w using Eq. (25)

$$g(t) = 16\pi^{-1}\int_0^1 w^2(1-w^2)^{\frac{1}{2}} \times \cos[w\omega_0(4N+6)^{\frac{1}{2}}t]\, dw \tag{30}$$

$$= -8\frac{d^2}{d\tau^2}[J_1(\tau)/\tau]|_{\tau=(4N+6)^{\frac{1}{2}}\omega_0 t}.$$

The integral $g(t)$ in Eq. (30) is a damped oscillating function of the time whose period is equal to $\pi\omega_0^{-1}N^{-\frac{1}{2}}$ and whose initial value $g(0)$ is equal to unity. It is clear that when the amplitude of the oscillating function $g(t)$ is comparable with $4N^{-1}+(8/3)\omega_0 t N^{-\frac{1}{2}}$, the function $g(t)$ does not provide any useful information concerning the autocorrelation function $\rho_N(t)$. This condition is reached at $t = \omega_0^{-1}N^{-1/10}$, where $g(\omega_0^{-1}N^{-1/10})$ is proportional to $N^{-3/5}$ and where $|g(\omega_0^{-1}N^{-1/10}) - \rho_N(\omega_0^{-1}N^{-1/10})| \leq (8/3)N^{-3/5}$. Consequently, we may conclude that

$$\rho_N(t) = -8(d^2/d\tau^2)[\tau^{-1}J_1(\tau)]|_{\tau=(4N+6)^{\frac{1}{2}}\omega_0 t} \quad \text{for } 0 \leq \omega_0 t \leq N^{-1/5}. \tag{31}$$

In this limited time interval, the difference $\rho_N(t) - g(t)$ satisfies the inequality,

$$|\rho_N(t) - g(t)| < 2N^{-7/10};$$

and in the neighborhood of $t = \omega_0^{-1}N^{-1/5}$, the amplitude of $\rho_N(\omega_0^{-1}N^{-1/5})$ is

$$2\pi^{-1/2}N^{-9/20},$$

a number which may be regarded effectively as zero, but which is nevertheless large compared to the upper bound of $|\rho_N(t) - g(t)|$. Thus, we have shown that, in a Bernoulli chain composed of $N+1$ identical particles, the momentum autocorrelation function of the top particle is approximated accurately by Eq. (31) in the time interval $0 < t < \omega_0^{-1}N^{-1/5}$. The difference between Eq. (31) and the exact value is less than $N^{-7/10}$ throughout the interval. The number $N^{-7/10}$ is small compared to the amplitude of oscillation of the autocorrelation function; and the amplitude of oscillation at $t = \omega_0^{-1}N^{-1/5}$ is $2\pi^{-\frac{1}{2}}N^{-9/20}$, which is effectively zero.

2. $\rho_0(t)$ When $\mathcal{Q} = 0$

The expression for $\rho_0(t)$ when $\mathcal{Q} = 0$ follows from Eq. (2) and is

$$\rho_0(t) = (N+1)^{-2}\sum_{\nu=1}^{N+1} k_\nu[L_N(k_\nu)]^{-2}\cos(\omega_0 k_\nu^{\frac{1}{2}}t). \tag{32}$$

The factor $[L_N(k_\nu)]^{-2}$ is a relatively smooth function of ν, since the maxima (or minima) of $L_N(k)$ are located near the k_ν's, the zeros of $L_{N+1}(k)$. The asymptotic formula for $[L_N(k_\nu)]^{-2}$ has been obtained in the Appendix, and its value is

$$[L_N(k_\nu)]^{-2} \sim \tfrac{1}{2}\pi N\left(\frac{k_\nu}{4N+6}\right)^{-\frac{1}{2}} \times \left(1 - \frac{k_\nu}{4N+6}\right)^{-\frac{1}{2}}\exp(-k_\nu). \tag{33}$$

[23] G. Polya and G. Szegö, *Aufgaben und Lehrsätze aus der Analysis* (Springer-Verlag, Berlin, 1964), 3rd ed., Vol. 1, p. 37.

Substitute Eq. (33) in (32) and obtain

$$\rho_0(t) = 2\pi \sum_{r=1}^{N+1} \left(\frac{k_r}{4N+6}\right)^{\frac{1}{2}} \left(1 - \frac{k_r}{4N+6}\right)^{-\frac{1}{2}} \exp(-k_r) \cos(\omega_0 k_r^{\frac{1}{2}} t). \tag{34}$$

Clearly, in Eq. (34) the high frequencies do not contribute significantly to $\rho_0(t)$ because of the presence of the factor $\exp(-k_r)$. With one minor modification, we proceed as in the case of $\rho_N(t)$ and introduce the integral $\mathcal{J}(t)$, for which the right-hand side of Eq. (34) is the discrete approximation,

$$\mathcal{J}(t) = \int_0^{\frac{1}{2}} 2\pi N w(\mu)[1 - w^2(\mu)]^{-\frac{1}{2}} \exp[-(4N+6)w^2(\mu)] \cos[\omega_0 w(\mu)(4N+6)^{\frac{1}{2}} t]\, d\mu, \tag{35}$$

where $w(\mu)$ and μ are defined as in Eq. (24). The minor change is in the upper limit of the integral. We omit the last $(1/2)N$ frequencies from the sum in (34) and the integral in (35). The contribution of these terms to $\rho_0(t)$ is negligible; and by excluding the point $\mu = 1$, the total variation of the integrand in Eq. (35) is finite. Thus, the magnitude of the difference $\rho_0(t) - \mathcal{J}(t)$ is

$$\begin{aligned} |\rho_0(t) - \mathcal{J}(t)| &\le \frac{1}{N+1} \int_0^{\frac{1}{2}} \left| \frac{d}{d\mu} \left\{ \frac{2\pi N w(\mu)}{[1 - w^2(\mu)]^{\frac{1}{2}}} \exp[-(4N+6)w^2(\mu)] \cos[(4N+6)^{\frac{1}{2}} \omega_0 t w(\mu)] \right\} \right| d\mu \\ &\le 2\pi \int_0^{\frac{1}{2}} \frac{dw(\mu)}{d\mu} \left\{ [1 - w^2(\mu)]^{-\frac{1}{2}} \left| \frac{d}{dw} (w(\mu) \exp[-(4N+6)w^2(\mu)]) \right| \right. \\ &\quad \left. + w(\mu) \exp[-(4N+6)w^2(\mu)] \left[\frac{(4N+6)^{\frac{1}{2}} \omega_0 t}{[1 - w^2(\mu)]^{\frac{1}{2}}} + \frac{w(\mu)}{[1 - w^2(\mu)]^{\frac{3}{2}}} \right] \right\} d\mu. \end{aligned} \tag{36}$$

When the independent variable is changed from μ to w in (36), the inequality can be written as

$$\begin{aligned} |\rho_0(t) - \mathcal{J}(t)| \le 2\pi \int_0^{w(\frac{1}{2})} \left\{ (1 - w^2)^{-\frac{1}{2}} \left| \frac{d}{dw} \{ w \exp[-(4N+6)w^2] \} \right| \right. \\ \left. + w \exp[-(4N+6)w^2] \left[\frac{(4N+6)^{\frac{1}{2}} \omega_0 t}{(1 - w^2)^{\frac{1}{2}}} + \frac{w}{(1 - w^2)^{\frac{3}{2}}} \right] \right\} dw \end{aligned}$$

or

$$\begin{aligned} |\rho_0(t) - \mathcal{J}(t)| &\le \frac{2\pi}{[1 - w^2(\tfrac{1}{2})]^{\frac{1}{2}}} \left\{ 2 \left[\frac{1}{2(4N+6)} \right]^{\frac{1}{2}} e^{-\frac{1}{2}} - w(\tfrac{1}{2}) \exp[-(4N+6)w^2(\tfrac{1}{2})] \right\} \\ &\quad + \frac{\pi \omega_0 t}{[1 - w^2(\tfrac{1}{2})]^{\frac{1}{2}}} \frac{1 - \exp[-(4N+6)w^2(\tfrac{1}{2})]}{(4N+6)^{\frac{1}{2}}} + 2\pi \frac{[1 - w^2(\tfrac{1}{2})]^{-\frac{3}{2}}}{(4N+6)^{\frac{1}{2}}} \int_0^{(4N+6)^{\frac{1}{2}} w(\frac{1}{2})} x^2 \exp(-x^2)\, dx, \end{aligned} \tag{37}$$

$$|\rho_0(t) - \mathcal{J}(t)| \le \frac{\pi}{[1 - w^2(\tfrac{1}{2})]^{\frac{1}{2}}} \left[\left(\frac{2}{e}\right)^{\frac{1}{2}} + \tfrac{1}{2}\omega_0 t \right] N^{-\frac{1}{2}}.$$

Thus the error made in replacing $\rho_0(t)$ by $\mathcal{J}(t)$ is at most $\backsim N^{-3/8}$ in the time interval $0 < t < \omega_0^{-1} N^{1/8}$. The integral $\mathcal{J}(t)$ is

$$\begin{aligned} \mathcal{J}(t) &= 8N \int_0^{w(\frac{1}{2})} w \exp[-(4N+6)w^2] \cos[(4N+6)^{\frac{1}{2}} \omega_0 t w]\, dw \\ &= 2 \int_0^{2N^{\frac{1}{2}} w(\frac{1}{2})} v \exp(-v^2) \cos(\omega_0 t v)\, dv. \end{aligned} \tag{38}$$

It can be seen in Eq. (38) that there is a negligible dependence of $\mathcal{J}(t)$ on N for $N \gg 1$. Therefore, we extend the range of integration to infinity and integrate by parts to obtain

$$\begin{aligned} \mathcal{J}(t) &= 1 - \omega_0 t \int_0^{\infty} \exp(-v^2) \sin(\omega_0 t v)\, dv \\ &= 1 - \omega_0 t \exp[-\tfrac{1}{4}\omega_0^2 t^2] \int_0^{\frac{1}{2}\omega_0 t} \exp(x^2)\, dx = 1 - \tfrac{1}{2}\omega_0^2 t^2 \exp[-\tfrac{1}{4}\omega_0^2 t^2]\, {}_1F_1[\tfrac{1}{2}, \tfrac{3}{2}; \tfrac{1}{4}\omega_0^2 t^2]. \end{aligned} \tag{39}$$

The initial value of $\mathcal{J}(t)$ in Eq. (39) is $\mathcal{J}(0) = 1$ and the asymptotic value[24] for $t \gg \omega_0^{-1}$ is

$$\mathcal{J}(t) \sim -2\omega_0^{-2}t^{-2}. \tag{40}$$

At intermediate values of t, it is readily verified from a table of numerical values of Dawson's integral,[25]

$$\exp(-x^2)\int_0^x \exp(y^2)\,dy,$$

that there is only one zero of $\mathcal{J}(t)$. This zero occurs for $t = 1.84\ \omega_0^{-1}$. For $t \sim \omega_0^{-1}N^{1/8}$, the value of $\mathcal{J}(t)$ is $\sim N^{-1/4}$. We therefore conclude that, in the time interval $0 < \omega_0 t < N^{1/8}$, the momentum autocorrelation function of the bottom particle in the Bernoulli chain is

$$\rho_0(t) = 1 - \omega_0 t \exp(-\tfrac{1}{4}\omega_0^2 t^2)\int_0^{\frac{1}{2}\omega_0 t} \exp(x^2)\,dx.$$

The error in $\rho_0(t)$ is at most $\sim N^{-3/8}$; and, except in the vicinity of the zero of $\rho_0(t)$, the magnitude is $\sim N^{-1/4}$ or greater.

It is also known that, in any system of coupled oscillators, $\rho_n(t)$ is the velocity of particle n at time t for a special initial condition of the entire harmonic oscillator system[15]: the condition in which all displacements and velocities are zero except for the unit velocity of particle n. Thus, the displacement of particle n at time t is the integral $\int_0^t \rho_n(\tau)\,d\tau$. In the present case, the maximum displacement of particle $n = 0$ occurs at $t = 1.84\ \omega_0^{-1}$ when the velocity is zero. Subsequently, the particle returns monotonically to its equilibrium position.

3. $\rho_N(t)$ When $1 \ll \mathcal{Q} \ll N$

The expression for $\rho_N(t)$ can be obtained by substituting Eq. (17) for $X_{N,\nu}$ in Eq. (1). The result can be written as

$$\rho_N(t) = \frac{4(1+\mathcal{Q})}{N+1}[1 + \tfrac{1}{2}(N+1)^{-1}] \times \sum_{\nu=1}^{N+1} \frac{\left(\frac{k_\nu}{4N+6}\right)\cos\left[\left(\frac{k_\nu}{4N+6}\right)^{\frac{1}{2}}\omega_0(4N+6)^{\frac{1}{2}}t\right]}{16\mathcal{Q}(\mathcal{Q}+1)[1+\tfrac{1}{2}(N+1)^{-1}]^2\left(\frac{k_\nu}{4N+6}\right)^2 - 8\mathcal{Q}[1+(N+1)^{-1}]\left(1+\frac{\mathcal{Q}}{N+1}\right)\left(\frac{k_\nu}{4N+6}\right) + \left(1+\frac{\mathcal{Q}}{N+1}\right)^2}, \tag{41}$$

where k_ν, $\nu = 1, \cdots, N+1$ are the $N+1$ zeros of the polynomial

$$\mathcal{O}_{N+1}(k) = (N+1)L_{N+1}(k) + \mathcal{Q}(1-k)L_N(k). \tag{42}$$

Because the zeros of $L_N(k)$ interlace the zeros of $L_{N+1}(k)$, it can be shown that a zero of $\mathcal{O}_{N+1}(k)$ is located between each pair of zeros of $L_{N+1}(k)$. In addition, $\mathcal{O}_{N+1}(k)$ has one root which is smaller than the smallest root of $L_{N+1}(k)$ when $\mathcal{Q} > 0$. Therefore, in the limit $N \gg 1$, the roots of $\mathcal{O}_{N+1}(k)$, when normalized to $4N+6$, fill the interval $(0, 1)$. Consequently, an integral can be constructed for which Eq. (41) is the discrete approximation. This integral is the analog of Eq. (30) for $\mathcal{J}(t)$ in the case of the perfect Bernoulli chain

$$\mathcal{K}(t) = 16\pi^{-1}(1+\mathcal{Q})\int_0^1 \frac{w^2(1-w^2)^{\frac{1}{2}}\cos[w\omega_0(4N+6)^{\frac{1}{2}}t]}{16\mathcal{Q}(\mathcal{Q}+1)w^4 - 8\mathcal{Q}w^2 + 1}\,dw. \tag{43}$$

It is readily verified that when $\mathcal{Q} = 0$, $\mathcal{K}(t)$ is equal to $\mathcal{J}(t)$. In deriving Eq. (43) we have assumed only that $N \gg 1$ and $0 < \mathcal{Q}/(N+1) \ll 1$. The magnitude of the difference $\rho_N(t) - \mathcal{K}(t)$ can be shown to satisfy the inequality

$$|\rho_N(t) - \mathcal{K}(t)| \le \frac{4(1+\mathcal{Q})}{N+1}\int_0^1 \left|\frac{d}{d\mu}\frac{w^2(\mu)\cos[w(\mu)\omega_0(4N+6)^{\frac{1}{2}}t]}{16\mathcal{Q}(\mathcal{Q}+1)w^4(\mu) - 8\mathcal{Q}w^2(\mu)+1}\right| d\mu$$

$$\le \frac{4}{N}\left\{\frac{\frac{1}{4}[(\mathcal{Q}+1)/\mathcal{Q}]^{\frac{1}{2}}}{1-[\mathcal{Q}/(\mathcal{Q}+1)]^{\frac{1}{2}}} - \frac{\mathcal{Q}+1}{16\mathcal{Q}+(4\mathcal{Q}-1)^2} + 2N^{\frac{1}{2}}\omega_0 t\int_0^1 \frac{(\mathcal{Q}+1)w^2\,dw}{16\mathcal{Q}(\mathcal{Q}+1)w^4 - 8\mathcal{Q}w^2+1}\right\}. \tag{44}$$

[24] A. Erdélyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 1, p. 278.

[25] *Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun, Eds. (National Bureau of Standards, Washington, D. C., 1964), p. 319.

When $\mathcal{Q} \gg 1$, the inequality (44) simplifies to

$$|\rho_N(t) - \mathcal{K}(t)| \leq 2\mathcal{Q}/N + (\pi/2N^{\frac{1}{2}})\omega_0 t. \quad (45)$$

This error bound is identical in form with that obtained in the case $\mathcal{Q} = 0$. Although we have not been able to evaluate $\mathcal{K}(t)$ in Eq. (43) in terms of known functions for arbitrary values of $\mathcal{Q} > 0$, we can evaluate $\mathcal{K}(t)$ in the limit $\mathcal{Q} \gg 1$.

The problem of evaluating $\mathcal{K}(t)$ in the limit $\mathcal{Q} \gg 1$ is relatively simple, because the factor

$$D(w) = 16(\mathcal{Q}+1)w^2[16\mathcal{Q}(\mathcal{Q}+1)w^4 - 8\mathcal{Q}w^2 + 1]^{-1}$$

has a very sharp and large maximum at $w_m = [16\mathcal{Q}(\mathcal{Q}+1)]^{-\frac{1}{4}} \cong (1/2)\,\mathcal{Q}^{-\frac{1}{4}}$. The value of $D(w_m)$ is

$$D(w_m) = 2[(\mathcal{Q}+1)/\mathcal{Q}]^{\frac{1}{2}}[1 - [\mathcal{Q}/(\mathcal{Q}+1)]^{\frac{1}{2}}]^{-1} \quad (46)$$

or

$$D(\tfrac{1}{2}\mathcal{Q}^{-\frac{1}{2}}) \cong 4\mathcal{Q}, \quad \text{for} \quad \mathcal{Q} \gg 1. \quad (47)$$

Start with the identity

$$\mathcal{K}(t) = \pi^{-1}\int_0^\infty D(w)\cos(w\tau)\,dw + \pi^{-1}\int_0^1 [(1-w^2)^{\frac{1}{2}} - 1]D(w)\cos(w\tau)\,dw - \pi^{-1}\int_1^\infty D(w)\cos(w\tau)\,dw, \quad (48)$$

where $\tau = (4N+6)^{\frac{1}{2}}\omega_0 t$. One can show for $\mathcal{Q} \gg 1$ that: (1) the second integral in Eq. (48) is less than $(\frac{5}{8} + 1/\pi)\,\mathcal{Q}^{-1}$ because the integrand is small at w_m; and (2) the third integral is less than $(\pi\mathcal{Q})^{-1}$ because w_m lies well outside the integration interval The first integral is a known cosine transform,[26] so one obtains

$$\mathcal{K}(t) = \mathcal{Q}^{-\frac{1}{4}}(\mathcal{Q}+1)^{\frac{1}{4}}\csc(2\theta) \times \sin\left[\theta - \frac{\tau\sin\theta}{2(\mathcal{Q}^2+\mathcal{Q})^{\frac{1}{2}}}\right]\exp\left[-\frac{\tau\cos\theta}{2(\mathcal{Q}^2+\mathcal{Q})^{\frac{1}{2}}}\right], \quad (49)$$

where

$$\cos 2\theta = -[\mathcal{Q}/(\mathcal{Q}+1)]^{\frac{1}{2}}.$$

In the limit $\mathcal{Q} \gg 1$ where $\sin\theta \cong 1$, $\cos\theta \cong (1/2)\,\mathcal{Q}^{-\frac{1}{2}}$, and $\theta \cong \pi/2 - (1/2)\,\mathcal{Q}^{-\frac{1}{2}}$, the expression for $\mathcal{K}(t)$ simplifies to

$$\mathcal{K}(t) = \exp[-N^{\frac{1}{2}}\omega_0 t/2\mathcal{Q}]\cos[N^{\frac{1}{2}}\omega_0 t/\mathcal{Q}^{\frac{1}{2}}]. \quad (50)$$

We therefore conclude that, in the time interval $0 < \omega_0 t < N^{-1/5}$, the momentum autocorrelation function of a very heavy particle at the top of a Bernoulli chain is

$$\rho_N(t) = \exp[-N^{\frac{1}{2}}\omega_0 t/2\mathcal{Q}]\cos[N^{\frac{1}{2}}\omega_0 t/\mathcal{Q}^{\frac{1}{2}}]. \quad (51)$$

The error in $\rho_N(t)$ arises from the replacement of $\rho_N(t)$ by $\mathcal{K}(t)$, and from the approximations made in evaluating $\mathcal{K}(t)$. The first of these errors is clearly small compared to $\rho_N(t)$ in the time interval $0 < \omega_0 t < N^{-1/5}$ when $N \gg \mathcal{Q} \gg 1$. The approximations made in evaluating $\mathcal{K}(t)$ limit the usefulness of the result to the sub-interval of $0 < \omega_0 t < N^{-1/5}$ in which $\rho_N(t)$ is appreciable compared to $\mathcal{Q}^{-1}$. When $N \gg 1$ there is no appreciable difference between $\rho_0(t)$ for $\mathcal{Q} = 0$ and $\rho_0(t)$ for $\mathcal{Q} \gg 1$.

D. SUMMARY AND REMARKS

We have shown that, in a perfect Bernoulli chain of $N+1$ particles ($\mathcal{Q} = 0$), the momentum autocorrelation functions of the top and bottom particles, $\rho_N(t)$ and $\rho_0(t)$, are radically different. In the former case, $\rho_N(t)$ decays in an oscillatory manner

$$\rho_N(t) = -8\frac{d^2}{d\tau^2}\left(\frac{J_1(\tau)}{\tau}\right)\Bigg|_{\tau=2N^{\frac{1}{2}}\omega_0 t}, \quad 0 \leq \omega_0 t < N^{-1/5}$$
$$\sim 8\left(\frac{2}{\pi}\right)^{\frac{1}{2}}\frac{\cos(2N^{\frac{1}{2}}\omega_0 t - \frac{3}{4}\pi)}{(2N^{\frac{1}{2}}\omega_0 t)^{\frac{3}{2}}}. \quad (52)$$

The amplitude of $\rho_N(t)$ in the neighborhood of $t = \omega_0^{-1}N^{-\frac{1}{4}}$ is $4\pi^{-\frac{1}{2}}N^{-\frac{1}{4}}$. In the latter case, $\rho_0(t)$ passes through zero only once (at $t \cong 1.84\,\omega_0^{-1}$) and approaches zero from below

$$\rho_0(t) = 1 - \tfrac{1}{2}\omega_0^2 t^2\exp[-\tfrac{1}{4}\omega_0^2 t^2]{}_1F_1[\tfrac{1}{2}, \tfrac{3}{2}; \tfrac{1}{4}\omega_0^2 t^2], \quad 0 \leq \omega_0 t < N^{\frac{1}{2}}$$
$$\sim -2\omega_0^{-2}t^{-2}, \quad \text{for} \quad t \gg \omega_0^{-1}.$$

The value of $\rho_0(t)$ when $t = \omega_0^{-1}N^{1/8}$ is $-2N^{-1/4}$. Thus it is seen that not only the forms of $\rho_N(t)$ and $\rho_0(t)$ are different, but the times $\omega_0^{-1}N^{-1/3}$ and $\omega_0^{-1}N^{1/8}$ at which the respective amplitudes decay to the value $N^{-1/4}$ are markedly different. In each case $\rho_N(t)$ and $\rho_0(t)$ are discrete cosine transforms based on the same normal mode frequency spectrum. The presence in the transform of the highest frequencies (which are proportional to $N^{\frac{1}{2}}$) is apparent in the form of $\rho_N(t)$ but not in that of $\rho_0(t)$. The greater weight of the high-frequency components in $\rho_N(t)$ and the more rapid damping of the decay envelope of $\rho_N(t)$ reflects the physical fact that the nearest-

[26] A. Erdelyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Tables of Integral Transforms* (McGraw-Hill Book Company, Inc., New York, 1954), Vol. 1, p. 9.

neighbor interaction or coupling constants are proportional to N in the vicinity of particle N. In the limit $N \to \infty$, the maximum frequency of the Bernoulli chain approaches infinity. To the authors' knowledge, there are only two investigations of systems of coupled harmonic oscillators in which infinite frequencies appear explicitly. These are a model of Brownian motion treated by Ford, Kac, and Mazur[17] and a model of an elastically bounded electron interacting with the electromagnetic field, treated by Ullersma.[18] In both investigations the case $N = \infty$ was considered. The transition $N \to \infty$ was not pertinent to the problems posed.

The properties of a heavy particle in a harmonic oscillator system are of interest in the theory of Brownian motion; and several systems have been studied.[2,3,7,9,13,15,27] In the remaining case, we have determined the time dependence of the top particle in a Bernoulli chain when the mass $m(1 + \mathcal{Q})$ of the top particle is large compared to the mass m of the other particles. The expression derived for $\rho_N(t)$ is characteristic of a classical Brownian oscillator. It can be written as

$$\rho_N(t) = \exp\left[-\Omega t/2\mathcal{Q}^{\frac{1}{2}}\right] \cos\left[\Omega t\right] + \delta(t), \tag{53}$$

where $\Omega = N^{\frac{1}{2}}\omega_0\mathcal{Q}^{-\frac{1}{2}}$ and where $\delta(t)$ satisfies an inequality of the form $|\delta(t)| < c\mathcal{Q}^{-1}$ with c of order unity. Thus, the first term in Eq. (53) is a useful approximation for $\rho_N(t)$ as long as $c\mathcal{Q}^{-1}$ is small compared to $\exp\left[-\Omega t/2\mathcal{Q}^{\frac{1}{2}}\right]$. It is clear from a comparison of Eq. (53) with (52) that the effect of increasing the mass of particle N is to inhibit the transfer of momentum between N and the rest of the chain. In addition, the effective frequency of oscillation is decreased. Similar behavior has been found in the case of a heavy isotope in a three-dimensional crystal model.[9]

APPENDIX

Consider the problem of calculating the asymptotic formula for $[L_N(k_\nu)]^{-2}$ when $N \gg 1$ and k_ν is a zero of $L_{N+1}(k)$. Using the asymptotic formula given in Eq. (21), the expression for $[L_N(k_\nu)]^{-2}$ can be written as

$$\begin{aligned}[L_N(k_\nu)]^{-2} &\sim \frac{\pi(N+\frac{1}{2})\sin\left[2\cos^{-1}\left(\frac{k_\nu}{4N+2}\right)^{\frac{1}{2}}\right]\exp\left(-k_\nu\right)}{\sin^2\left\{(2N+1)\left[\cos^{-1}\left(\frac{k_\nu}{4N+2}\right)^{\frac{1}{2}} - \left(\frac{k_\nu}{4N+2}\right)^{\frac{1}{2}}\left(1-\frac{k_\nu}{4N+2}\right)^{\frac{1}{2}}\right] + \frac{1}{4}\pi\right\}} \\ &\sim \frac{\pi(2N+1)w_\nu\left(\frac{4N+6}{4N+2}\right)^{\frac{1}{2}}\left[1 - w_\nu^2\left(\frac{4N+6}{4N+2}\right)\right]^{\frac{1}{2}}\exp\left[-(4N+6)w_\nu^2\right]}{\sin^2\left((2N+1)\left\{\cos^{-1}\left[w_\nu\left(\frac{4N+6}{4N+2}\right)^{\frac{1}{2}}\right] - w_\nu\left(\frac{4N+6}{4N+2}\right)^{\frac{1}{2}}\left[1-w_\nu^2\left(\frac{4N+6}{4N+2}\right)\right]^{\frac{1}{2}}\right\} + \frac{1}{4}\pi\right)}.\end{aligned} \tag{A1}$$

Equation (A1) can be simplified by expanding the factors containing $[(4N + 6)/(4N + 2)]$ in powers of N^{-1}

$$[(4N+6)/(4N+2)]^{\frac{1}{2}} \cong 1 + 1/2N, \tag{A2}$$

$$\cos^{-1}\{w_\nu[(4N+6)/(4N+2)]^{\frac{1}{2}}\} \cong \cos^{-1} w_\nu - (2N)^{-1}w_\nu(1-w_\nu^2)^{-\frac{1}{2}}, \tag{A3}$$

$$\{1 - w_\nu^2[(4N+6)/(4N+2)]\}^{\frac{1}{2}} \cong (1-w_\nu^2)^{\frac{1}{2}} - (2N)^{-1}w_\nu^2(1-w_\nu^2)^{-\frac{1}{2}}, \tag{A4}$$

and introducing the factor $2N + 3$ in the argument of the sine function. The result is

$$[L_N(k_\nu)]^{-2} \sim \frac{2N\pi w_\nu(1-w_\nu^2)^{\frac{1}{2}}\exp\left[-(4N+6)w_\nu^2\right]}{\sin^2\left\{(2N+3)[\cos^{-1} w_\nu - w_\nu(1-w_\nu^2)^{\frac{1}{2}}] - 2\cos^{-1} w_\nu + \frac{1}{4}\pi\right\}}. \tag{A5}$$

But, from the definition of k_ν, we have for $N \gg 1$

$$\sin^2\{(2N+3)[\cos^{-1} w_\nu - w_\nu(1-w_\nu^2)^{\frac{1}{2}}] + \tfrac{1}{4}\pi - 2\cos^{-1} w_\nu\} = \sin^2(2\cos^{-1} w_\nu) = 4w_\nu^2(1-w_\nu^2). \tag{A6}$$

Therefore the asymptotic formula for $[L_N(k_\nu)]^{-2}$ reduces to

$$[L_N(k_\nu)]^{-2} \sim \tfrac{1}{2}N\pi w_\nu^{-1}(1-w_\nu^2)^{-\frac{1}{2}}\exp\left[-(4N+6)w_\nu^2\right]. \tag{A7}$$

[27] R. J. Rubin, J. Am. Chem. Soc. 86, 3413 (1964).

Some Remarks on the Construction of Invariants of Semisimple Local Lie Groups

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A general form of the l invariants of compact semisimple local Lie groups or rank l, as the traces of the powers of the "velocity potential" operator is suggested. The connection of this form of the invariants with those of Ref. 3 is described. The possible generalization beyond those of adjoint group and its connection with that of Biedenharn is discussed.

SEVERAL attempts have been made[1-3] in recent years to obtain the invariants of semisimple local Lie groups. They all consist in generalizing Racah-type invariants and to show that there are only l independent invariants for a group of rank l. Such invariants have been constructed in the earlier literature for the special case of adjoint groups[4]. The inadequacy of these invariants, especially to suit the covariant and contravariant representations, has been pointed out in Ref. 1. The object of this paper is to show that the nth-order invariants of the semisimple local Lie group of rank l can be expressed as the nth-power spur of the velocity-potential U operator of the group of infinitesimal generators. Also, it is shown that since this velocity potential operator has always an expansion in terms of the self-representation of the infinitesimal generators, one can always choose the self-representation for the infinitesimal generators without loss of generality. The connection of the present work with that of Ref. 3 is given. The tensor behavior of U is pointed out. We essentially follow the treatment of Ref. 4 for notation and subject.

Since we are going to deal with the "velocity potential" of the adjoint group, let us first introduce its properties here. The "velocity potential" is defined to be

$$U^i_\alpha(x) = [\partial\phi_i(x, y)/\partial y_\alpha]_{y=0}, \tag{1}$$

where the ϕ's are the transformation functions of the Lie group. In fact, as is well known, the whole analysis and the classification of continuous groups are accomplished by the study of U. The infinitesimal generators of the group X are defined by

$$X_\rho = \sum_i U^i_\rho(x) \frac{\partial}{\partial x_i}. \tag{2}$$

The functions ϕ are analytic and have an expansion

$$\phi_\alpha(x, y) = x_\alpha + y_\alpha + a^\alpha_{\beta\gamma}x_\beta y_\gamma + fx^2y + \cdots. \tag{3}$$

The structure constants of the group $C^\alpha_{\beta\gamma}$ are related to a's through the relation

$$c^\alpha_{\beta\gamma} = a^\alpha_{\beta\gamma} - a^\alpha_{\gamma\beta}. \tag{4}$$

These concepts are indeed well known and are introduced just for continuity and notation. The U operator for the group 0(3), for example, looks like

$$U^i_\rho(x) = \begin{pmatrix} 0 & +z & -y \\ -z & 0 & x \\ y & -x & 0 \end{pmatrix}, \quad x_i = (x, y, z). \tag{5}$$

The adjoint group P of a group G is defined through the homomorphism of G on the group of matrices. So, to every element $x \in G$, there corresponds a matrix $p \in P$. The adjoint group of the infinitesimal group is called the infinitesimal adjoint group.

Let us start with the Casimir operator

$$\begin{aligned} I_2 &= g_{\alpha\beta}X^\alpha X^\beta \\ &= C^{\sigma_1}_{\alpha\sigma_2}C^{\sigma_2}_{\beta\sigma_1}X^\alpha X^\beta. \end{aligned} \tag{6}$$

Now, if we want to express this as a trace which could later be generalized, we naturally introduce the concept of a matrix. This association is sometimes achieved by taking the adjoint representation in which

$$C^{\sigma_1}_{\alpha\sigma_2} = \begin{pmatrix} A \\ X_\alpha \end{pmatrix}^{\sigma_1}_{\sigma_2}, \tag{7}$$

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[1] L. C. Biedenharn, J. Math. Phys. 4, 436 (1963).

[2] M. Umezawa, Nucl. Phys. 48, 111 (1963). For similar connected work, also refer to: M. Micu, Nucl. Phys. 60, 353 (1964); A. M. Perelomov and V. S. Popov, Soviet Phys.—JETP Letters 1, 6 (1965); and F. Halbwachs, CERN preprint 65/1585/5(TH.617).

[3] B. Gruber and L. O'Raifeartaigh, J. Math. Phys. 5, 1796 (1964). See also, for a detailed discussion: L. O'Raifeartaigh, *Lectures on Local Lie Groups and Their Representations*, MATSCIENCE Report 25 (The Institute of Mathematical Sciences, Madras, India).

[4] L. P. Eisenhart, *Continuous Groups of Transformations* (Dover Publications, Inc., New York, 1961), Chap. IV, p. 155. See also L. C. Biedenharn, *Lectures in Theoretical Physics*, W. E. Brittin, B. W. Downs, and J. Downs, Eds. (Interscience Publishers, Inc., New York, 1963), Vol. 5, pp. 347–349.

so that I_2 can be expressed as

$$I_2 = \mathrm{Tr}\begin{pmatrix} A & A \\ X_\alpha & X_\beta \end{pmatrix} X^\alpha X^\beta. \tag{8}$$

We then look to replace the adjoint representation by some general representation, so that when I_2 is generalized, it is really independent of the choice of the representation. What we want to emphasize is that we need essentially an association (whether with adjoint representation or otherwise) of (CX) with a matrix in order to express I_2 as a trace. In other words, if we define

$$\eta^{\sigma_1}_{\sigma_3} = C^{\sigma_1}_{\alpha\sigma_3} X^\alpha, \tag{9}$$

then

$$I_2 = \mathrm{Tr}\,(\eta)^2, \tag{10}$$

so that the generalized nth-order invariant may just be written as

$$I_n = \mathrm{Tr}\,(\eta)^n. \tag{11}$$

These are, of course, known as the invariants of the adjoint group (see Ref. 4 for extensive information). The invariants are defined as the coefficients in the expansion of the characteristic equation

$$\Delta(X, \rho) = \det\,(\eta^\alpha_i(X) - \rho\,\delta^\alpha_b) = 0, \tag{12}$$

as powers of ρ. The parameter ρ is supposed to define the invariant directions. The Killing theorem states that the coefficients ψ in the characteristic equation of the group

$$\Delta(X, \rho) = \rho^\gamma - \psi_1(X)\rho^{\gamma-1} + \cdots + (-1)^{\gamma-1}\psi_{\gamma-1}(X)\rho, \tag{13}$$

are in fact the invariants of the adjoint group. Also it has been shown that there are only l independent ψ's where l is the rank of the group. The operator $\eta(X)$ is just the operator $(X \leq \hat{X})$ defined in Ref. 3. These are velocity potential operators for the group of the infinitesimal generators X of the group. For the case of 0(3), the operator η is obtained by replacing, in the velocity potential $U(x)$ of the group, the elements of the group by the infinitesimal generators. So, for 0(3) we get

$$\eta = \begin{bmatrix} 0 & X_3 & -X_2 \\ -X_3 & 0 & X_1 \\ X_2 & -X_1 & 0 \end{bmatrix} = {}_*U(X), \tag{14}$$

which is in fact the operator $(X \times \hat{X})$ of Ref. 3. The invariants of the group are then

$$I_n = \mathrm{Tr}\begin{bmatrix} 0 & X_3 & -X_2 \\ -X_3 & 0 & X_1 \\ X_2 & -X_1 & 0 \end{bmatrix}^n. \tag{15}$$

It is easy to show that, for 0(3), $I_3 = f(I_2)$, so that there is only one Casimir operator for 0(3).

Therefore, the method consists of first replacing the x's in the U matrix of the group [defined through Eq. (1)] by the infinitesimal generators of the group [defined in Eq. (2)]. Then take the traces of the powers of this new matrix. It is clear that the number of X's is indeed equal to the order of the group. It is also easy to see that trace $(U)^n$ is the same even if one permutes the X's in U. Of course, the choice of $U(X)$ strongly indicates that the corresponding group function is

$$\phi'_\alpha(X, Y) = C^\alpha_{\beta\gamma} X_\beta Y_\gamma,$$

so that

$$U^\alpha_i(X) = \left[\frac{\partial \phi'_\alpha}{\partial Y_i}\right]_{Y=0} = C^\alpha_{\beta i} X_\beta,$$

and hence

$$\begin{aligned} I_2 &= \mathrm{tr}\,(U)^2 \\ &= U^\alpha_i U^i_\alpha \\ &= g_{\beta\gamma} X_\beta X_\gamma. \end{aligned}$$

The form of $U^\alpha_\beta(X)$, and hence that of $\phi'_\alpha(X, Y)$ immediately tells us that we are in fact dealing with the invariants of the adjoint group.

Since $U(X)$ is a transformation function, it can be shown to be a tensor operator. We will not discuss the completeness of these invariants and their explicit construction for special cases. These problems have been discussed in Ref. 3.

Finally, it may be worthwhile to point out that if we want to generalize these invariants beyond the adjoint group, we can still retain the form

$$I_n = \mathrm{Tr}\,(U)^n.$$

But now, U's are defined through the relation

$$U^\alpha_i = a^\alpha_{\beta i} X_\beta,$$

where a's are not the structure constants. They are the second-order coefficients occurring in the expansion of ϕ'_α for the general case. We know, however, that the structure constants are related to the a's by the relation

$$\begin{aligned} C^\alpha_{\beta\gamma} &= a^\alpha_{\beta\gamma} - a^\alpha_{\gamma\beta} \\ &= \text{antisymmetric part.} \end{aligned}$$

Usually, in the normal parameter system, we make the symmetric part of a vanish so that a's, occurring in the expansion of ϕ', can be replaced by the structure constants. The generalization of the general invariants beyond those of adjoint group consists in retaining both the symmetric and antisymmetric parts of a; in other words, having the general expansion for ϕ'. In this case,

$$a^{\alpha}_{\beta\gamma} = \tfrac{1}{2}(a^{\alpha}_{\beta\gamma} + a^{\alpha}_{\gamma\beta}) + \tfrac{1}{2}(a^{\alpha}_{\beta\gamma} - a^{\alpha}_{\gamma\beta})$$
$$= \tfrac{1}{2}(d^{\alpha}_{\beta\gamma} + c^{\alpha}_{\beta\gamma}),$$

where $d^{\alpha}_{\beta\gamma}$ are symmetric structure constants occurring in the anticommutator of the X's,

$$\{X_\alpha, X_\beta\} = d^{\gamma}_{\alpha\beta}X_\gamma,$$

and C's are the usual structure constants (antisymmetric) occurring in the commutator of the X's,

$$[X_\alpha, X_\beta] = C^{\gamma}_{\alpha\beta}X_\gamma.$$

So, to conclude, the generalization of I_n beyond the adjoint group is found to be

$$I_n = \mathrm{Tr}\,(U)^n,$$
$$U^i_\alpha = a^i_{\alpha\gamma}X_\gamma; \qquad a^i_{\alpha\gamma} = \tfrac{1}{2}(d^i_{\alpha\gamma} + C^i_{\alpha\gamma}).$$

Incidentally, the a's are used by Biedenharn[1] to construct the general invariants I_n.

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