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Method to Obtain the Character Tables of Nonsymmorphic Space Groups

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A method is developed to obtain the character tables of nonsymmorphic space groups. The method is based on the possibility of obtaining all the irreducible representations of a group, if one knows all the irreducible representations of its invariant subgroup of index 2 or 3. It turns out that all the space groups have an invariant subgroup of index 2 or 3.

INTRODUCTION

THERE exists a simple method to obtain the character tables of the irreducible representations of symmorphic space groups.[1] However, more than 150 space groups are nonsymmorphic and it is more difficult to obtain the character tables of their irreducible representations.

Döring and Zehler[2] show in their paper how to obtain the character tables of a nonsymmorphic group in the case of a diamond. In principle, this method can be used also for other nonsymmorphic space groups,[3,4] but in each case one has to construct artificially a new group, find its irreducible representations, and choose from them the suitable ones.

In this paper we develop a general method to obtain the character tables of the irreducible representations of all nonsymmorphic space groups.

We first give a short introduction on concepts and results of the theory of groups, which have not been used until now in applications in physics.

Let G be a finite group and H its subgroup of index m. We can write

$$G=H+v_1H+v_2H+\cdots+v_{m-1}H. \qquad (1)$$

The elements $v_1, v_2, \cdots, v_{m-1}$ are called representing elements of the group G relative to the subgroup H. If the subgroup H has the property that $u^{-1}Hu=H$, where u is any element of G, then H is called an invariant subgroup. The cosets $H, v_1H, \cdots, v_{m-1}H$ in (1) are then elements of a new group, called factor group of G. The order of the factor group is equal to the index of the subgroup H. It is known that every subgroup of index 2 is an invariant one and every factor group relative to a subgroup of index 3 is a cyclic one. In the last case we can write the group in the following way:

$$G=H+vH+v^{-1}H=H_0+H_1+H_2. \qquad (2)$$

The element H_0 is the unit element of the factor group and the other two elements H_1 and H_2 are inverse to each other, i.e., $H_1H_2=H_0$, $H_1^2=H_2$, and $H_2^2=H_1$.

Let s be an element of the subgroup H (from now on s will always be an element of H). If H is an invariant subgroup, then all the elements of the class generated by the element s will belong to H. It can happen that the class of the element s in G is split in H into several classes, i.e., the elements $u^{-1}su$, where u is any element of G and belongs to different classes in H.

If H is an invariant subgroup of index 2, then either the class r of an element s in G is not split in H at all, or it is split into two classes with the same number of elements. The first case happens when some element of the class r commutes with an element which does not belong to H. The second case happens if no element of the class r commutes with an element which does not belong to H.[5]

[1] G. Koster, Solid State Physics **5**, 173 (1957).
[2] W. Döring and V. Zehler, Ann. Physik **13**, 214 (1953).
[3] U. Firsof, JETP (U.S.S.R.) **32**, 1350 (1957).
[4] E. Kashba, Solid State (U.S.S.R.) **1**, 407 (1959).
[5] F. D. Murnaghan, Theory of Group Representations (Johns Hopkins Press, Baltimore, 1938), p. 168.

In the same way one can prove that if H is an invariant subgroup of index 3, the class r of the element s in G either is not split at all in H, or is split into three classes with the same number of elements, $n_r/3$.

Let us now define a characteristic of a finite group G. Let Γ_j be an irreducible representation of G with characters $\chi_j^{(1)}, \chi_j^{(2)}, \cdots, \chi_j^{(p)}$, and F^k—a class function, i.e., F has the same values F^k for all elements of G, which belong to the same class k. The expression

$$\phi_j=\frac{1}{g}\sum_k n_k F^k \chi_j^{(k)*}$$

is called the simple characteristic of G, where g is the order of the group G and n_k is the number of elements in class k; the sum includes all the classes of G. If the representation in the definition of the characteristic ϕ_j is reducible, the characteristic is termed a compound characteristic of G. The coefficients of any one of the indeterminates (e.g., F^k) in ϕ_j yield, when multiplied by g and divided by n_k, the complex conjugate of the character of the representation Γ_j, which is associated with the class k.

In the same way we can define a simple characteristic of H:

$$\varphi_j=\frac{1}{h}\sum_k n_k' f^k \xi_j^{(k)*}. \tag{3}$$

It is known (p. 98 of work cited in footnote 5) that if one identifies the indeterminates in Eq. (3), associated with all those classes of H, which belong to the same class of G, then Eq. (3) is a characteristic (in general, a compound one) of G. Therefore, every irreducible representation γ_j of the subgroup H furnishes a representation Γ (in general a reducible one) of the group G. The character $\chi^{(i)}$ of such a representation of G, which corresponds to the class i, is equal to the conjugate of the sum of the coefficients of the indeterminates f in Eq. (3) associated with all those classes of H, which belong to the same class i of G, multiplied by g and divided by n_i

$$\chi^{(i)}=\frac{g}{hn_i}\sum_k n_k' \xi^{(k)}. \tag{4}$$

The sum in (4) includes all classes of H, which belong to the same class i of G. The dimension of the representation Γ is equal to the character $\chi^{(1)}$ which corresponds to the unit element. Therefore, it is equal to the dimension of the γ_j by which Γ is furnished, multiplied by g/h. If H is an invariant subgroup, then the characters (4) that correspond to elements, which do not belong to H, are null (p. 93 of work cited in footnote 5).

I. A METHOD TO OBTAIN ALL THE IRREDUCIBLE REPRESENTATIONS OF A FINITE GROUP, WHEN ONE KNOWS ALL THE IRREDUCIBLE REPRESENTATIONS OF AN INVARIANT SUBGROUP OF INDEX 2 OR 3

We first develop the method for the case of an invariant subgroup of index 2.

Let H be a subgroup of index 2 and let $\xi_1, \xi_2, \cdots \xi_k$ be the characters of all the irreducible representations $\gamma_1, \gamma_2, \cdots \gamma_k$ of H. The simple characteristics $\varphi_1, \varphi_2, \cdots, \varphi_k$ of H furnish representations of G with characters [according to (4)],

$$\chi^{(r)}=\frac{g}{hn_r}\sum_l n_l' \xi_j^{(l)}=\frac{2}{n_r}\sum_l n_l' \xi_j^{(l)}. \tag{6}$$

The representations of G, which are furnished by all the simple characteristics $\varphi_1, \varphi_2, \cdots \varphi_k$ of H must include all the irreducible representations of G. Indeed, we cannot assume that some irreducible representation (e.g., Γ_m) of G is not included in these representations because Γ_m as a representation of H can be written in the following way: $\Gamma_m=\sum_k c_k\gamma_k$, where at least one coefficient (e.g., c_1) must differ from zero. According to the Frobenius theorem (p. 100 of work cited in footnote 5) the representation of G, which is furnished by the simple characteristic φ_1 of H, must include the irreducible representation Γ_m.

When H is a subgroup of index 2, then n_l' in (6) is equal either to n_r or to $n_r/2$, and (6) can be written

$$\chi^{(r)}=\xi_j(s)+\xi_j(v^{-1}sv),$$

where v is an element which does not belong to H. By using the definition of conjugate representation, we have

$$\chi^{(r)}=\xi_j(s)+\bar{\xi}_j(s). \tag{7}$$

We can divide all the irreducible representations of H into two sets: a set of pairs of conjugate nonequivalent representations and a set of self-conjugate representations (p. 100 of work cited in footnote 5). We now construct the irreducible representations of G, which are included in the representations of G furnished by the two sets of representations of H, and in such a way we obtain all the irreducible representations of G.

Theorem 1. Let γ_k and its conjugate $\bar{\gamma}_k$ be two irreducible and nonequivalent representations of H. The representation Γ_k of G, which is furnished by γ_k (or by $\bar{\gamma}_k$) is an irreducible representation of G. Its order is twice the order of γ_k.

Proof. From (7) we see that the representations γ_k and $\bar{\gamma}_k$ furnish the same representation of G, because the representation, which is conjugate to $\bar{\gamma}_k$, is γ_k. The order of Γ_k is twice the order of γ_k because $(g/h)=2$. We must

still prove that Γ_k is irreducible. One has

$$\sum_G|\chi_k|^2=\sum_H|\xi_k(s)+\bar{\xi}_k(s)|^2$$
$$=\sum_H|\xi_k(s)|^2+2\sum_H\xi_k(s)\bar{\xi}_k(s)^*$$
$$+\sum_H|\bar{\xi}_k(s)|^2=h+0+h=2h=g,$$

i.e., Γ_k is irreducible. Therefore, every pair of conjugate representations of H furnishes an irreducible representation of G.

Let us take now two different pairs of conjugate and nonequivalent representations of H: γ_i, $\bar{\gamma}_i$ and γ_k, $\bar{\gamma}_k$.

The representations Γ_i and Γ_k of G, which are furnished by them are nonequivalent because

$$\sum_G\chi_i\chi_k^*=\sum_H(\xi_i+\bar{\xi}_i)(\xi_k+\bar{\xi}_k)^*$$
$$=\sum_H\xi_i\bar{\xi}_k+\sum_H\xi_i\bar{\xi}_k^*+\sum_H\bar{\xi}_i\bar{\xi}_k+\sum_H\bar{\xi}_i\bar{\xi}_k^*=0.$$

If H contains n pairs of conjugate irreducible and nonequivalent representations, they furnish n irreducible nonequivalent representations of G.

Let us now prove the following theorem: Let γ_m be a self-conjugate irreducible representation of H. The representation of G, which is furnished by γ_m, is reducible and contains two irreducible and nonequivalent representations Γ_m', Γ_m'' of G. Their order is equal to the order of γ_m and their characters on H are equal to those of γ_m.

Proof: from (7) we have for the characters χ_m of Γ_m,

$$\chi_m=\xi_m+\bar{\xi}_m=2\xi_m. \tag{8}$$

Moreover,

$$\sum_G|\chi_m|^2=\sum_H|2\xi_m|^2=4\sum_H|\xi_m|^2=4h=2g.$$

Therefore, Γ_m contains two irreducible representations of G, because 2 can be written only in one way as a sum of squares: $2=1^2+1^2$. We can write $\Gamma_m=\Gamma_m'+\Gamma_m''$. Both Γ_m' and Γ_m'' as representations of H contain the representation γ_m (according to the theorem of Frobenius), and therefore they have the same characters as γ_m on H, because the order of Γ_m is twice the order of γ_m. We must still prove that Γ_m' and Γ_m'' are nonequivalent.

Let v be an element which does not belong to H. The element vs then does not belong to H and from

$$\chi_m(vs)=\chi_m'(vs)+\chi_m''(vs)=0$$

we have

$$\chi_m'(vs)=-\chi_m''(vs). \tag{9}$$

But Γ_m' is irreducible, and therefore

$$g=\sum_G|\chi_m'|^2=\sum_H|\chi_m'(s)|^2+\sum_H|\chi_m'(vs)|^2$$
$$=h+\sum_H|\chi_m'(vs)|^2$$

(the last sum includes the elements that do not belong to H). We obtain

$$\sum_H|\chi_m'(vs)|^2=g-h=h. \tag{10}$$

By using (9) and (10) and the fact that the representations Γ_m' and Γ_m'' have equal characters on H, we get

$$\sum_G\chi_m'\chi_m''^*=\sum_H\chi_m'(s)\chi_m''^*(s)+\sum_H\chi_m'(vs)\chi_m''(vs)^*$$
$$=\sum_H|\chi_m'(s)|^2-\sum_H|\chi_m'(vs)|^2=h-h=0,$$

i.e., Γ_m' and Γ_m'' are nonequivalent. Therefore every self-conjugate irreducible representation of H furnishes two irreducible and nonequivalent representations of G.

Let us take now two different irreducible self-conjugate representations, γ_l and γ_m of H. The representations Γ_l', Γ_l'' and Γ_m', Γ_m'' of G, which are furnished by them, are all nonequivalent. Indeed, every pair of representations Γ_l', Γ_l'' and Γ_m', Γ_m'' are nonequivalent according to the previous proof; the representations Γ_m' and Γ_l' (the same holds for the other representations) are also nonequivalent; otherwise their characters on H would be equal and they would be furnished by the same representation of H.

Therefore, if H contains m self-conjugate irreducible and nonequivalent representations, they furnish $2m$ irreducible and nonequivalent representations of G.

It is also clear that no representation of G, which is furnished by the m self-conjugate representations of H, is equivalent to any representation of G furnished by one of the pairs of conjugate nonequivalent representations of H. Otherwise, they would be furnished by the same representation of H.

Therefore, the n pairs of conjugate nonequivalent representations and the m self-conjugate representations of H furnish $n+2m$ irreducible and nonequivalent representations of G and these are all the irreducible representations of G.

Let us now deal with the characters of these representations. The characters of the representations, which are furnished by the pairs of conjugate representations of H, are obtained by (7) as a sum of the characters associated with the same element in the two representations γ_k and $\bar{\gamma}_k$. (It is clear that the character associated with elements which do not belong to H are zero).

The characters of the representations Γ_m' and Γ_m'' of G on H are equal to those of γ_m (by which they are furnished). The characters associated with elements which do not belong to H can be obtained from the following argument. Let v be an element which does not belong to H. v^2 is then an element of H, say s. The character associated with $v^2=s$ in Γ_m' and Γ_m'' is known. Let the scalar matrix $A(v)$, the square of the character of which is equal to the character of s in γ_m, be associated with the element v and the matrix $A(v)A(t)$—with the element vt of G, which does not belong to H ($A(t)$ is the matrix, associated with the element t of H in the representation γ_m). The two sets of matrices $A(t)$; $\pm A(v)A(t)$ in which matrices $A(t)$ of γ_m are associated with elements of H and matrices $\pm A(v)A(t)$—with element vt, are two irreducible, nonequivalent representations Γ' and Γ'' of G. In fact, as the diagonal element of the matrix $A(v)$ must be a root of the unit

(G is a finite group) we have

$$|\chi'(vt)|^2=|\chi'(t)|^2;\quad |\chi''(vt)|^2=|\chi''(t)|^2,$$

and therefore

$$\sum_G|\chi'|^2=\sum_H|\chi'(t)|^2+\sum_H|\chi'(vt)|^2=2h=g. \quad (11)$$

The same holds for the characters χ'' of Γ''. From the definition of Γ' and Γ'', it follows

$$\chi'(t)=\chi''(t);\quad \chi'(vt)=-\chi''(vt),$$

and therefore

$$\sum_G\chi'\chi''^*=\sum_H\chi'(t)\chi''(t)^*+\sum_H\chi'(vt)\chi''(vt)^*=0. \quad (12)$$

Equations (11) and (12) show that Γ' and Γ'' are irreducible and nonequivalent representations. It is clear that Γ' and Γ'' must be equivalent to Γ_m' and Γ_m'', respectively, because they have the same characters on H and only two nonequivalent representations are furnished by γ_m. Therefore, the characters of Γ_m' and Γ_m'' associated with an element vt which does not belong to H are

$$\chi(vt)=\pm Z\xi_m(t)=\pm\left(\frac{1}{l}\xi_m(v^2)\right)^{\frac{1}{2}}\cdot\xi_m(t), \quad (13)$$

where $\chi(vt)$ are the characters of Γ_m', Γ_m'', Z is the element of the diagonal of the scalar matrix $A(v)$, $\xi_m(t)$ is the character of γ_m, and l the order of γ_m.

We now develop the method for the case of an invariant subgroup of index 3. If we define two conjugate representations $\bar\gamma_j$ and $\bar\gamma_j'$ to the representation γ_j by means of elements v and v^{-1} of (2), we can write in this case the expression (4) as

$$\chi^{(r)}=\xi_j(s)+\bar\xi_j(s)+\bar\xi_j'(s). \quad (14)$$

Let us prove that if $\bar\gamma_j$ is equivalent to γ_j, then $\bar\gamma_j'$ is also equivalent to γ_j, and all the three representations are equivalent and vice versa; if $\bar\gamma_j$ and γ_j are nonequivalent, then all the three representations γ_j, $\bar\gamma_j$ and $\bar\gamma_j'$ are nonequivalent. Indeed, let $A(s)$ and $A(v^{-1}sv)$ be matrices of equivalent (nonequivalent) representations γ_j and $\bar\gamma_j$. If we construct conjugate representations to γ_j and $\bar\gamma_j$ by means of the element v, we obtain the representations $\bar\gamma_j$ and $\bar\gamma_j'$, respectively. It is clear that if γ_j and $\bar\gamma_j$ are equivalent (nonequivalent) then $\bar\gamma_j$ and $\bar\gamma_j'$ will also be equivalent (nonequivalent). Now let us construct conjugate representations to γ_j and $\bar\gamma_j$ by means of v^{-1}. We obtain the representations $\bar\gamma_j'$ and γ_j, respectively. If γ_j and $\bar\gamma_j$ are equivalent (nonequivalent), $\bar\gamma_j'$ and γ_j will also be equivalent (nonequivalent). Therefore, the three representations γ_j, $\bar\gamma_j$, and $\bar\gamma_j'$ are either all equivalent or all nonequivalent and we can divide all the irreducible representations of H into two sets: a set of triads of conjugate nonequivalent representations and a set of self-conjugate representations. We can again prove as in the case of a subgroup of index 2 that if H contains n triads of conjugate representations and m self-conjugate representations, they furnish $n+3m$ irreducible and nonequivalent representations of G.

The characters of the representations furnished by a triad of conjugate representations of H are equal, according to (14), to the sum of the characters associated with the same element in the three representations γ_j, $\bar\gamma_j$, and $\bar\gamma_j'$ (the characters associated with elements which do not belong to H are zero). For the characters of the representations of G, which are furnished by the self-conjugate representations of H, we have:

$$\begin{aligned}&\text{for element of } H \quad \chi(t)=\xi_m(t)\\ &\text{for element of } vH \quad \chi(vt)=(1)^{\frac{1}{2}}Z\xi_m(t)\\ &\text{for element of } vH \quad \chi(v^{-1}t)=[(1)^{\frac{1}{2}}Z]^{-1}\xi_m(t).\end{aligned} \quad (15)$$

Here $Z=[(1/l)\xi_m(v^3)]^{\frac{1}{2}}$ and l is the order of γ_m. The formulas (13) and (15) hold in the case when it is possible to associate with an element of G which does not belong to H a scalar matrix. This case is important in applications to space groups.

II. CHARACTER TABLES OF NONSYMMORPHIC SPACE GROUPS

Any element of a space group can be written as $\{\alpha|\mathbf{a}\}$ (see p. 176 of work cited in footnote 1) where α is an element of a point group and $\mathbf{a}$ is a translation. The space group is a symmorphic one if it contains together with every element $\{\alpha|\mathbf{a}\}$ also the elements $\{\alpha|0\}$ and $\{e|\mathbf{a}\}$ (e is the unit of the point group). If some element $\{\alpha|\mathbf{a}\}$ belongs to the space group, but the elements $\{\alpha|0\}$ and $\{e|\mathbf{a}\}$ do not, the space group is nonsymmorphic.

Every space group can be represented by m cosets (1) relative to the subgroup of translations H.

$$G=\{e|0\}H+\{\alpha_1|\mathbf{a}_1\}H+\cdots+\{\alpha_{m-1}|\mathbf{a}_{m-1}\}H. \quad (16)$$

In a symmorphic group we are able to choose the representing elements

$$\{e|0\},\ \{\alpha_1|\mathbf{a}_1\},\ \cdots\{\alpha_{m-1}|\mathbf{a}_{m-1}\} \quad (17)$$

in such a way, that they are all pure elements of a point group and form by themselves a group. This cannot be done for a nonsymmorphic group and this is the reason of the difficulty in obtaining the character tables of nonsymmorphic groups.

In order to be able to use the method of the previous section, we have to know all the irreducible representations of an invariant subgroup of index 2 or 3 of the space group. The character tables of symmorphic groups can be obtained in a simple way and if a nonsymmorphic space group contains an invariant symmorphic subgroup of index 2 or 3, the problem is solved at once by our method. More than 100 nonsymmorphic groups contain an invariant symmorphic subgroup of index 2 and only

4 $(C_3^2, C_3^3, C_6^4, C_6^5)$[6] an invariant symmorphic subgroup of index 3.

In order to show how to use our method for the other nonsymmorphic groups, let us first note that all space groups contain an invariant subgroup of index 2 or 3. This is a consequence of the fact that all point groups contain an invariant subgroup of index 2 or 3 (as one can easily verify). Indeed, if a set of point group elements

$$e, \alpha_1, \cdots \alpha_f \tag{18}$$

of the representing elements (17) forms an invariant subgroup of index 2 or 3 of the point group

$$e, \alpha_1, \cdots \alpha_{m-1}, \tag{19}$$

then the set F of elements,

$$F=\{e|0\}H+\{\alpha_1|\mathbf{a}_1\}H+\cdots+\{\alpha_f|\mathbf{a}_f\}H \tag{20}$$

is an invariant subgroup of index 2 or 3 of the whole group G(16).

TABLE I. Symmetry points in the Brillouin zone and the corresponding subgroups of 0_h^2 and T^4.

	K_x	K_y	K_z	Representing elements of the subgroups of 0_h^2	Representing element of the subgroups of T^4
Γ	0	0	0	All the elements (21)	All the elements (22)
R	$\frac{\pi}{a}$	$\frac{\pi}{a}$	$\frac{\pi}{a}$	All the elements (21)	All the elements (22)
X	0	$\frac{\pi}{a}$	0	E, C_4^{2z}, C_4^{2y}, C_4^{2x}, C_4^{y}, C_4^{3y}, C_2^{xy0}, $C_2^{\bar{x}y0}$ and their products with P	E, $\left\{C_4^{2z}\middle\vert\frac{a}{2}\frac{a}{2}0\right\}\left\{C_4^{2y}\middle\vert0\frac{a}{2}\frac{a}{2}\right\}$ $\left\{C_4^{2z}\middle\vert\frac{a}{2}0\frac{a}{2}\right\}$
M	$\frac{\pi}{a}$	$\frac{\pi}{a}$	0	E, C_4^{2z}, C_4^{2y}, C_4^{2x}, C_4^{x}, C_4^{3x}, C_2^{xy0}, $C_2^{\bar{x}y0}$ and their products with P	E, $\left\{C_4^{2z}\middle\vert\frac{a}{2}\frac{a}{2}0\right\}\left\{C_4^{2y}\middle\vert0\frac{a}{2}\frac{a}{2}\right\}$ $\left\{C_4^{2z}\middle\vert\frac{a}{2}0\frac{a}{2}\right\}$
Δ	0	K_y	0	E, C_4^{2y}, C_4^{y}, C_4^{3y}, PC_4^{2x}, PC_4^{2z}, PC_2^{xoz}, $PC_2^{\bar{x}oz}$	E, $\left\{C_4^{2y}\middle\vert0\frac{a}{2}\frac{a}{2}\right\}$
Σ	K_x	K_x	0	E, C_2^{xy0}, PC_4^{2z}, $PC_2^{\bar{x}y0}$	E
Λ	K_x	K_x	K_x	E, C_3^{xyz}, C_3^{2xyz}, $PC_2^{\bar{x}y0}$, $PC_2^{\bar{x}oz}$, $PC_2^{o\bar{y}z}$	E, $\{C_3^{xyz}\vert0\,0\,0\}$, $\{C_3^{2xyz}\vert0\,0\,0\}$
T	$\frac{\pi}{a}$	$\frac{\pi}{a}$	K_z	E, C_4^{2z}, C_4^{z}, C_4^{3z}, PC_4^{2z}, PC_4^{2y}, PC_2^{xy0}, $PC_2^{\bar{x}y0}$	E, $\left\{C_4^{2z}\middle\vert\frac{a}{2}0\frac{a}{2}\right\}$
Z	K_x	$\frac{\pi}{a}$	0	E, C_4^{2z}, PC_4^{2z}, PC_4^{2y}	E, $\left\{C_4^{2z}\middle\vert\frac{a}{2}\frac{a}{2}0\right\}$
S	K_x	$\frac{\pi}{a}$	K_x	E, C_2^{xoz}, PC_4^{2y}, $PC_2^{\bar{x}oz}$	E
$\Sigma\Lambda$	K_x	K_x	K_x	E, PC_2^{xy0}	E
$\Delta\Sigma$	K_x	K_y	0	E, PC_4^{2z}	E
A	$\frac{\pi}{a}$	K_y	K_z	E, PC_4^{2z}	E

[6] *International Tables for X-Ray Crystallography* (Kynoch Press, Birmingham, England, 1952), Vol. 1, pp. 250, 278, 279; a. *ibid.*, p. 307.

Therefore, we can use our method as follows. If an invariant subgroup of a nonsymmorphic space group is also nonsymmorphic, we have first to find the character tables of the nonsymmorphic subgroup. This can be done at once if the nonsymmorphic subgroup has an invariant symmorphic subgroup of index 2 or 3. If not, we repeat this process once more and so on until we obtain an invariant symmorphic subgroup of index 2 or 3. Only for a few nonsymmorphic space groups we must repeat this process three times.

As an illustration to our method let us find the character tables of the space groups 0_h^2 and T^4 for the symmetry points in $\mathbf{k}$ space. The group 0_h^2 has an invariant symmorphic subgroup of index 2. This is the group 0^1. Let

$$P=\left\{I\middle\vert\frac{a}{2}\frac{a}{2}\frac{a}{2}\right\}$$

be an element which contains the inversion and a translation by a vector

$$\left(\frac{a}{2}\frac{a}{2}\frac{a}{2}\right).$$

The representing elements of 0_h^2 relative to the subgroup of translations then are all the elements of the point group 0 and the products of its elements with the element P:

$$0, P0. \tag{21}$$

The representing elements of T^4 relatively to the subgroup of translations are[6a]

$$\begin{array}{lll}
\{E|0\,0\,0\} & \{C_3^{xyz}|0\,0\,0\} & \{C_3^{2xyz}|0\,0\,0\} \\
\left\{C_4^{2x}\middle\vert\frac{a}{2}\frac{a}{2}\frac{a}{2}\right\} & \left\{C_3^{\bar{x}y\bar{z}}\middle\vert\frac{a}{2}\frac{a}{2}0\right\} & \left\{C_3^{2\bar{x}y\bar{z}}\middle\vert\frac{a}{2}0\frac{a}{2}\right\} \\
\left\{C_4^{2y}\middle\vert0\frac{a}{2}\frac{a}{2}\right\} & \left\{C_3^{\bar{x}\bar{y}z}\middle\vert0\frac{a}{2}\frac{a}{2}\right\} & \left\{C_3^{2\bar{x}\bar{y}z}\middle\vert\frac{a}{2}\frac{a}{2}0\right\} \\
\left\{C_4^{2z}\middle\vert\frac{a}{2}0\frac{a}{2}\right\} & \left\{C_3^{x\bar{y}\bar{z}}\middle\vert\frac{a}{2}0\frac{a}{2}\right\} & \left\{C_3^{2x\bar{y}\bar{z}}\middle\vert0\frac{a}{2}\frac{a}{2}\right\},
\end{array} \tag{22}$$

where C_4^{2x} is a rotation about the x axis by π; similarly, C_4^{2y}, C_4^{2z}; C_3^{xyz}, C_3^{2xyz}—are rotations about an axis in the direction (111) by 120° and 240°; the other elements C_3 have a similar meaning.

Let us now write Table I, which will contain the symmetry points in the Brillouin zone and the corresponding subgroups of 0_h^2 and T^4 (we denote the symmetry points as in the paper by Bouckaert, Smoluchowski and Wigner,[7] hereafter referred to as BSW). The element C_2^{xy0} in the Table I means a rotation about the direction (110) by π. A similar meaning is attached to the other elements C_2.

[7] L. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. 50, 58 (1936).

TABLE II. Characters of the irreducible representations of the point group 0.

0	E	$8C_3$	$3C_4^2$	$6C_2$	$6C_4$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
F_2	3	0	−1	1	−1
F_1	3	0	−1	−1	1

TABLE III.[a] Characters of the subgroup of 0_h^2 corresponding to the point R.

R	E	$8C_3$	$3C_4^2$	$6C_2$	$6C_4$	P	$8PC_3$	$3PC_4^2$	$6PC_2$	$6PC_4$
R_1	2	2	2	0	0	0	0	0	0	0
R_2	6	0	−2	0	0	0	0	0	0	0
R_3	2	−1	2	0	0	2	−1	2	0	0
R_4	2	−1	2	0	0	−2	1	−2	0	0

[a] In Tables III–X the characters for the representing elements are given.

We now begin to obtain the character tables by 0_h^2. The tables for the symmetry points Γ, Δ, Σ, Λ, $\Sigma\Lambda$, $\Delta\Sigma$, inside the Brillouin zone are the same as in the paper by BSW; one has only, for elements $\{\alpha|\mathbf{a}\}$, to multiply the character of α by $e^{i\mathbf{k}\mathbf{a}}$ (see p. 223 of work cited in footnote 1).

To the points on the surface of the Brillouin zone correspond groups which have invariant symmorphic subgroups of index 2. In order to obtain the character tables for them we have to write the character tables for the representing elements of the invariant symmorphic subgroup of index 2 to determine the conjugate and the self-conjugate representations and to construct the character tables of the group according to the method of the previous section. Let us do it for the point R. The representing elements of the symmorphic subgroup are the elements of the point group 0. The characters of 0 are given in Table II.[8]

In order to find which of the representations in Table II are conjugate and which self-conjugate let us find the connection between the characters $\chi(\alpha)$ and $\chi(P^{-1}\alpha P)$ for the point R (α is an element of 0 and

$$P=\left(I\left|\begin{matrix}a&a&a\\-&-&-\\2&2&2\end{matrix}\right.\right),$$

$$P^{-1}EP=E; \qquad \chi(P^{-1}EP)=\chi(E)$$

$$P^{-1}C_3^{xyz}P=\{C_3^{xyz}|0\,0\,0\}; \quad \chi(P^{-1}C_3P)=\chi(C_3)$$

$$P^{-1}C_4^{2x}P=\{C_4^{2x}|0\;a\;a\};$$

$$\chi(P^{-1}C_4^2P)=\exp\left[i\left(\begin{matrix}\pi&\pi\\-&-\\a&a\end{matrix}\right)a\right]\chi(C_4^2)=\chi(C_4^2)$$

$$P^{-1}C_2^{xy0}P=\{C_2^{xy0}|0\,0\;a\};$$

$$\chi(P^{-1}C_2P)=\exp\left(\begin{matrix}\pi\\i-a\\a\end{matrix}\right)\chi(C_2)=-\chi(C_2)$$

$$P^{-1}C_4^zP=\{C_4^z|0\;a\;0\};$$

$$\chi(P^{-1}C_4P)=\exp\left(\begin{matrix}\pi\\i-a\\a\end{matrix}\right)\chi(C_4)=-\chi(C_4).$$

From the connection between the characters one sees that there are two pairs A_1, A_2, and F_1, F_2 of conjugate representations and one self-conjugate E. We obtain, therefore, 4 irreducible representations for the point R: two representations (one of the order 2 and one of the order 6) furnished by the two pairs A_1, A_2 and F_1, F_2 of conjugate representations and two representations of order 2 furnished by the self-conjugate representations E. The characters of the first two representations are equal to the sum of the characters associated with the same element in the conjugate representations (formula 7). The characters of the two representations (R_3, R_4 in Table III), which are furnished by E, are equal to the characters of E for the elements of 0; for the elements $P\alpha$ we obtain according to (13): $\chi(P\alpha)=\pm\chi(\alpha)$ because $P^2=E$ ($E-$unit) and $\chi(P^2)=l$. Therefore, the character table for the point R is Table III.

In a similar way we obtain the character tables for the other points (Tables IV–VII).

Let us now obtain the character tables for the representing elements of T^4. We shall write tables only for the symmetry points on the surface of Brillouin zone. The groups of the points T and Z have invariant symmorphic subgroups of index 2 (the group of translations) and for them we obtain the character tables as for the group 0_h^2. For the points X and M we have to use our method twice and for the point R three times. Let us construct in detail the character table for the point R. The group of the point R has an invariant nonsymmorphic subgroup of index 3 [the first column in (22) with all translations]. We denote this subgroup by

TABLE IV. Characters of the subgroup of 0_h^2 corresponding to the points X and M.

M	X	E E	$C_4^{3x}C_4^{2x}$ $C_4^{3x}C_4^{2y}$	C_4^{2y} C_4^{3z}	$C_2^{xy0}C_2^{\bar{x}y0}$ $C_4^zC_4^{3z}$	$C_4^yC_4^{3y}$ $C_2^{xy0}C_2^{\bar{x}y0}$	P P	$PC_4^{2x}PC_4^{2z}$ $PC_4^{2x}PC_4^{2y}$	PC_4^{2y} PC_4^{2z}	$PC_2^{xy0}PC_2^{\bar{x}y0}$ $PC_4^zPC_4^{3z}$	$PC_4^yPC_4^{3y}$ $PC_2^{xy0}PC_2^{\bar{x}y0}$
M_1	X_1	2	0	2	0	2	0	0	0	0	0
M_2	X_2	2	0	2	0	−2	0	0	0	0	0
M_3	X_3	2	0	−2	0	0	2	0	−2	0	0
M_4	X_4	2	0	−2	0	0	−2	0	2	0	0

[8] L. Landau and E. Lifshitz, "Quantum mechanics" (Pergamon Press, London-Paris, 1958), p. 339 (translated).

H. It has a nonsymmorphic invariant subgroup of index 2 [the two first elements of the first column in (22) with all translations]. We denote it by F. The group F has an invariant symmorphic subgroup of index 2 (the group of translations) and the characters for the representing elements of F are in Table VIII because

$$\left\{C_4^{2x}\left|\frac{a}{2}\frac{a}{2}0\right.\right\}^2=\{E|a\,0\,0\}$$

and

$$\chi\left[\left\{C_4^{2x}\left|\frac{a}{2}\frac{a}{2}0\right.\right\}^2\right]=\chi\{E|a\,0\,0\}=\exp[i(\pi/a)a]=-1.$$

In order to obtain the character table for the representing elements of H, let us note that we can write H as follows:

$$H=F+\left\{C_4^{2y}\left|0\frac{a}{2}\frac{a}{2}\right.\right\}F.$$

The representations F_1 and F_2 in Table VIII are conjugate because

$$\left\{C_4^{2y}\left|0\frac{a}{2}\frac{a}{2}\right.\right\}^{-1}\left\{C_4^{2x}\left|\frac{a}{2}\frac{a}{2}0\right.\right\}\left\{C_4^{2y}\left|0\frac{a}{2}\frac{a}{2}\right.\right\}$$

$$=\left\{C_4^{2x}\left|-\frac{a}{2},-\frac{a}{2},a\right.\right\}=\left\{C_4^{2x}\left|\frac{a}{2}\frac{a}{2}0\right.\right\}\{E|-a,\,a,\,-a\}$$

TABLE V. Characters of the subgroup of O_h^2 corresponding to the point T.

	E	$C_4^zC_4^{3z}$	C_4^{2z}	P	$PC_4^{3x}PC_4^{2y}$	$PC_2^{xy0}PC_2^{\bar{x}y0}$
T_1	2	0	2	0	0	0
T_2	2	0	−2	0	0	0

TABLE VI. Character of the subgroup of O_h^2 corresponding to the points Z and S.

Z	E	C_4^{2z}	PC_4^{2y}	PC_4^{2z}
S	E	C_2^{x0z}	PC_4^{2y}	$PC_2^{\bar{x}0z}$
	2	0	0	0

TABLE VII. Characters of the subgroup of O_h^2 corresponding to the point A.

A	E	PC_4^{2x}
A_1	1	$\exp\left[\frac{i}{2}(k_y+k_z)a\right]$
A_2	1	$\exp\left[-\frac{i}{2}(k_y+k_z)a\right]$

TABLE VIII. Characters of the subgroup F.

	E	$\left\{C_4^{2x}\left\|\frac{a}{2}\frac{a}{2}0\right.\right\}$
F_1	1	i
F_2	1	$-i$

TABLE IX. Characters of the subgroup H.

E	$\left\{C_4^{2x}\left\|\frac{a}{2}\frac{a}{2}0\right.\right\}$	$\left\{C_4^{2y}\left\|0\frac{a}{2}\frac{a}{2}\right.\right\}$	$\left\{C_4^{2z}\left\|\frac{a}{2}0\frac{a}{2}\right.\right\}$
2	0	0	0

TABLE X. Characters of the subgroup of T^4 corresponding to the point R.

R	E	C_3^{xyz}	C_3^{2xyz}	$\left(C_4^{2z}\left\|\frac{a}{2}\frac{a}{2},0\right.\right)$
R_1	2	−1	−1	0
R_2	2	$-\exp\left(\frac{2\pi i}{3}\right)$	$-\exp\left(\frac{4\pi i}{3}\right)$	0
R_3	2	$-\exp\left(\frac{4\pi i}{3}\right)$	$-\exp\left(\frac{2\pi i}{3}\right)$	0

and the character

$$\chi\left[\left\{C_4^{2y}\left|0\frac{a}{2}\frac{a}{2}\right.\right\}^{-1}\left\{C_4^{2x}\left|\frac{a}{2}\frac{a}{2}0\right.\right\}\left\{C_4^{2y}\left|0\frac{a}{2}\frac{a}{2}\right.\right\}\right]$$

$$=\exp\left[ia\left(-\frac{\pi}{a}+\frac{\pi}{a}-\frac{\pi}{a}\right)\right]\chi\left\{C_y^{2x}\left|\frac{a}{2}\frac{a}{2}0\right.\right\}$$

$$=-\chi\left\{C_4^{2x}\left|\frac{a}{2}\frac{a}{2}0\right.\right\}.$$

Therefore, for the representing elements of H, we obtain Table IX.

From here it is easy to find the character table for the point R of the group T^4 if we note that

$$T^4=H+C_3^{xyz}H+C_3^{2xyz}H.$$

As $(C_3^{xyz})^3=E$ we have in the expression (15) $Z=1$, and therefore it is easy to write the character table for R (Table X).

Note that we have actually obtained the character tables for all symmetry points on the surface of the Brillouin zone. In fact, Table IX corresponds to points X and M and Table VIII to points T and Z.

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Problem of Rainich for Two-Component Spinors*

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Some general relations for two-component spinors in general relativity are derived in an attempt to solve the problem of Rainich for this case. A set of algebraic equations allows us in principle to express the current vector in terms of the energy-momentum tensor, and thus in terms of the Einstein tensor, but we have not succeeded in solving these equations except in a special frame of reference. Weyl's equations are expressed in terms of the current vector, its derivatives, and the energy-momentum tensor. In the last chapter, the determination of the spinor variables themselves is studied.

1. INTRODUCTION

THIS paper is concerned with a study of classical two-component spinors in the covariant formalism, and we will adhere, with some exceptions, to the notation of Infeld and van der Waerden[1]: spinor indices which may assume the values one or two will be denoted by greek letters α, β, $\cdots$, and a dotted index indicates that the transformations of the spinor with respect to this index have to be performed with the conjugate complex transformation coefficient: in particular, we will assume that a spinor with dotted indices replaced by undotted one's and vice versa, is equal to the conjugate complex of the original spinor. The metric tensor g_{nm} reduces in a galilean frame of reference to $g_{00}=1$ and $g_{11}=g_{22}=g_{33}=-1$.

The fundamental equations are Einstein's equation,

$$R_{nm}-\tfrac{1}{2}g_{nm}R=-T_{nm} \tag{1}$$

with

$$T_{nm}=i\{\sigma_n{}^{\dot\alpha\beta}(\psi_{\dot\alpha;m}\psi_\beta-\psi_{\dot\alpha}\psi_{\beta;m}) +\sigma_m{}^{\dot\alpha\beta}(\psi_{\dot\alpha;n}\psi_\beta-\psi_{\dot\alpha}\psi_{\beta;n})\} \tag{2}$$

and Weyl's equations,[2]

$$W^\beta=\sigma^{n\dot\alpha\beta}\psi_{\dot\alpha;n}=0 \tag{3}$$

$$W^{\dot\alpha}=\sigma^{n\dot\alpha\beta}\psi_{\beta;n}=0, \tag{3'}$$

where $\sigma^{n\dot\alpha\beta}$ are the generalized Pauli matrices. They are hermitean, i.e., $\sigma^{n\dot\alpha\beta}$ is the conjugate complex of $\sigma^{n\dot\beta\alpha}$, and satisfy

$$\gamma_{\dot\alpha\dot\mu}(\sigma^{n\dot\alpha\beta}\sigma^{m\dot\mu\nu}+\sigma^{m\dot\alpha\beta}\sigma^{n\dot\mu\nu})=2g^{nm}\gamma^{\beta\nu}, \tag{4}$$

as well as

$$\sigma^{n\dot\alpha\beta}\sigma_n{}^{\dot\mu\nu}=2\gamma^{\dot\alpha\dot\mu}\gamma^{\beta\nu}. \tag{5}$$

Here, $\gamma_{\alpha\beta}$ is the alternating spinor[3]

$$\gamma_{\alpha\beta}=-\gamma_{\beta\alpha}, \tag{6}$$

$\gamma^{\alpha\beta}$ is defined by

$$\gamma^{\alpha\beta}\gamma_{\alpha\mu}=\delta^\beta{}_\mu, \tag{7}$$

and similarly for the dotted alternating spinor $\gamma_{\dot\alpha\dot\beta}$. The two Kronecker spinors $\delta^\alpha{}_\beta$ and $\delta^{\dot\alpha}{}_{\dot\beta}$ are both equal to unity if their indices are equal, and otherwise they vanish. The alternating spinors are used to lower and raise spinor indices according to the convention

$$\psi_\alpha=\gamma_{\beta\alpha}\psi^\beta;\quad \psi^\alpha=\gamma^{\alpha\beta}\psi_\beta, \tag{8}$$

where the second equation is, of course, a consequence of the first, and the order of the indices has to be kept in mind.

The covariant differentiation indicated by a semicolon in Eqs. (2) and (3) will be specified later. We only mention that covariant derivation of any tensor shall be understood here as being formed with the ordinary Christoffel brackets. These quantities are also used to form the Einstein tensor in Eq. (1).

The specific form of the left hand side of the Einstein equations, however, will not concern us greatly in this work. Most of our studies will hold also in the presence of other physical systems, which possess energy and momentum, provided these systems do not interact with our spinor field. We could use instead of Eq. (1),

$$R_{nm}-\tfrac{1}{2}g_{nm}R+\theta_{nm}=-T_{nm}, \tag{9}$$

and add to Eq. (3) other field equations which control the variables on which θ_{nm} may depend, but a dependence of θ_{nm} on ψ_α or $\psi_{\dot\alpha}$ is specifically excluded in the following considerations.

2. OUTLINE OF THE PROBLEM

The recent progress in the theory of elementary particles has established the usefulness of the two-component theory for the description of neutrinos. Stimulated by this progress, Brill and Wheeler[4] carried out a theoretical study of the two-component neutrinos in the gravitational field. The present paper has little bearing on these physical problems. The purpose of this work is to carry out the Rainich procedure for

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[1] L. Infeld and B. L. van der Waerden, Preuss. Akad. Wiss. (1933), p. 380.

[2] H. Weyl, Z. Physik **56**, 330 (1929); see also W. Pauli, *Encyclopedia of Physics* (Springer Verlag, Berlin, 1958), Vol. V/1, p. 149.

[3] Not a spinor density. We will not use Infeld and van der Waerden's alternative approach.

[4] D. R. Brill and J. A. Wheeler, Revs. Modern Phys. **29**, 465 (1957); see also P. G. Bergmann, Phys. Rev. **107**, 624 (1957).

the simplest spinor field.[5] We formulate our program as follows: to find the necessary and sufficient conditions for the Einstein tensor[6] to be equal to the energy-momentum tensor of a two-component neutrino field in an arbitrary space-time domain. By assuming we know the Einstein tensor, we can then decide at once whether its nonvanishing is caused by the presence of neutrinos. More ambitiously, we can try to find an explicit representation of the spinor field in terms of "geometrical" quantities, like the metric tensor and the Einstein tensor. The Weyl equations will then appear as differential equations in terms of the geometrical quantities and the spinor would appear superfluous. Such a program is obviously subject to some limitations; for example, a constant phase factor of ψ_α remains arbitrary both in Einstein's and Weyl's equations, and cannot possibly be determined. Also, the phrase "geometrical" quantities needs further clarification. We cannot hope to represent the spinor ψ_α in terms of tensors and must expect the appearance of $\sigma^{n\dot{\alpha}\beta}$ and of $\gamma_{\alpha\beta}$ and other derived spinors. Regardless of how geometrical these quantities may appear from a mathematical viewpoint, they certainly lack any geometrical significance in terms of rods and clocks. In particular, we hope to determine the spinor only up to an arbitrary spinor transformation, and the latter is less physical than a coordinate transformation. These spinor transformations still do not exhaust the arbitrariness. The generalized Pauli matrices are fixed by Eqs. (4) and (5) only up to a sign, and the transitions from the one to the other are not equivalent to a spinor transformation. Or, we can say that there is no spinor transformation which compensates the changes in the σ's due to a reflection of any one coordinate.

If we ignore these unavoidable ambiguities for the moment, the solution of our problem would give the unification of neutrino fields and the gravitational field in the same sense as Rainich's unification of electromagnetism and gravitation. The main point in favor of these unified theories is their conservative feature. Even if the unification does not lead to an altogether new picture of the universe, at least a classical theory has been looked upon from a different angle, and this may deepen the understanding of an old picture.

There is one other aspect worth mentioning. We cannot easily insulate space-time domains against neutrinos, and the energy-momentum contributions resulting from neutrinos are to a certain extent unavoidable and uncontrollable. One might eventually have use for a "phenomenological" Einstein theory, in which only controllable energy and momentum enter; in other words, a suitable average of the Einstein theory over unknown contributions, as for instance, neutrinos.

3. CURRENT VECTOR

To avoid the ambiguities as far as possible, it appears advantageous to study the tensors associated with the spinors. One is led immediately to consider the current vector

$$J^n=\sigma^{n\dot{\alpha}\beta}\psi_{\dot{\alpha}}\psi_\beta \tag{10}$$

with the property

$$J^nJ_n=0. \tag{11}$$

By choosing the Pauli matrices in a local galilean frame of reference, we can see that this vector determines ψ_α up to a phase factor at the point under consideration. We now introduce a geodesic frame. The 16 ordinary differential quotients $J^n{}_{,m}$ are not independent and do not determine $\psi_{\alpha,m}$. In fact, four more quantities are needed to fix the components of the gradient of the phase factor. These four quantities can be obtained from the energy-momentum tensor (as a rule, the diagonal elements will suffice) which is supposed to be known, since it is equal to a geometrical quantity. We conclude that J^n and $J^n{}_{,m}$ suffice to determine ψ_α and $\psi_{\alpha,m}$ at a fixed point up to a phase constant.

Since the differential quotients $\psi_{\alpha,m}$ are restricted by Weyl's equations,[7] we expect more differential conditions on $J^n{}_{,m}$ and possibly the energy-momentum tensor.

Somewhat surprisingly, it is possible to derive covariant algebraic relations for J^n, which hold independently of Weyl's equations and involve, besides J^n, only the geometrical quantities g_{nm}, R_{nm}, and $R_{nm;p}$.[8] They allow us in principle to calculate J^n everywhere, and thus to calculate their derivatives, although we have not succeeded in doing this explicitly. They certainly imply some limitations on the Einstein tensor, but, again, we have been unable to formulate them covariantly. We defer the problem of how to calculate the spinors from these relations, and give now their derivations.

We state first a representation of the alternating tensor density ϵ^{nmpq} in terms of the σ

$$\epsilon^{nmpq}=\tfrac{1}{4}i(-g)^{\frac{1}{2}}(\sigma^{n\dot{\alpha}\beta}\sigma^{m\dot{\mu}\nu}-\sigma^{m\dot{\alpha}\beta}\sigma^{n\dot{\mu}\nu})\sigma^p{}_{\dot{\mu}\beta}\sigma^q{}_{\dot{\alpha}\nu}. \tag{12}$$

The proof of this representation is straightforward in a particular frame of reference. We introduce the tensor

$$U_{nm}=\sigma_n{}^{\dot{\alpha}\beta}(\psi_{\dot{\alpha};m}\psi_\beta-\psi_{\dot{\alpha}}\psi_{\beta;m}), \tag{13}$$

whose symmetric part is essentially the tensor T_{nm}

$$T_{nm}=i(U_{nm}+U_{mn}), \tag{14}$$

[5] The Rainich procedure was originally developed for the electromagnetic field coupled to the gravitational field: G. Y. Rainich, Trans. Am. Math. Soc. **27**, 106 (1925); G. W. Misner and J. A. Wheeler, Ann. Physik **2**, 525 (1957); L. Witten, Phys. Rev. **115**, 206 (1959); see also D. Sharp, Phys. Rev. Letters **3**, 108 (1959).

[6] Or rather the sum of the Einstein tensor and a possible additional tensor θ_{nm} as explained in connection with Eq. (9).

[7] These restrictions on the $\psi_{\alpha,m}$ are still not sufficient to express $\psi_{\alpha,m}$ in terms of $J^n{}_{,m}$ without also using some components of the energy-momentum tensor.

[8] O. Bergmann and L. Witten, Bull. Am. Phys. Soc. **3**, 368 (1958).

and derive

$$\epsilon^{nmpq}U_{qr}J_p=i(-g)^{\frac{1}{2}}(J^mJ^n{}_{;r}-J^nJ^m{}_{;r}). \quad (15)$$

The next step is the derivation of

$$T_{nm}J^nJ^m=0 \quad (16)$$

from Eq. (2), and this is quite elementary. For further reference we note here also

$$T_{nm;p}J^nJ^mJ^p=0, \quad (17)$$

but we will not derive this equation now. Obviously, Eqs. (11), (16), and (17) do not suffice to determine J^n.

Since Eq. (16) holds identically, we may differentiate it

$$J^nJ^mT_{nm;q}=-2J^n{}_{;q}J^mT_{nm} \quad (18)$$

and we multiply this equation with $J^rT_{pr}\epsilon^{pqst}J_s$, and replace $J^n{}_{;q}J_s$ by

$$J^n{}_{;q}J_s=J_{s;q}J^n-i(-g)^{-\frac{1}{2}}\epsilon^n{}_{vws}U^w{}_qJ^v \quad (19)$$

because of Eq. (15). The first term of the right-hand side in Eq. (19) will not contribute in Eq. (18) because of Eq. (16) and we get

$$\epsilon^{pqst}J_sJ^rT_{pr}J^nJ^mT_{nm;q}=2i(-g)^{-\frac{1}{2}}J^rT_{pr}J^mT_{nm}\epsilon^{pqst}\epsilon^{nvw}{}_sU_{wq}J_v. \quad (20)$$

We use now the well-known expansion formula for the product of the ϵ densities, and omit at once terms containing g^{pv}. The right-hand side of Eq. (20) reduces even more if we use also

$$J_nU^{nm}=0, \quad (21)$$

and thus

$$iU^{nm}J_m=T^{nm}J_m. \quad (22)$$

Consequently, we obtain for the right-hand side of Eq. (20)

$$2i(-g)^{-\frac{1}{2}}J^tJ^nT_{pn}J^mT_{qm}(U^{pq}-g^{pq}U^s{}_s). \quad (23)$$

By inserting into Eq. (20) and expressing U^{nm} by T^{nm}, we get finally

$$J^t=\frac{\epsilon^{pqst}J_sJ^rT_{pr}J^nJ^mT_{nm;q}}{(-g)^{\frac{1}{2}}J^nT_{pn}J^mT_{qm}(T^{pq}-g^{pq}T)}, \quad (24)$$

where the trace of the energy-momentum tensor

$$T=T^s{}_s \quad (25)$$

vanishes because of Weyl's equations. We may replace the energy-momentum tensor by the Einstein tensor—assuming that no other physical systems are present—and obtain relations between J^n and geometrical quantities.

We have not succeeded in solving for J^n explicitly, but the following considerations clarify the contents of Eq. (24) sufficiently. First we notice that Eqs. (11), (16), and (17) are actually contained in Eq. (24) and that there is only one further equation, Eq. (24), of interest. Whereas Eqs. (11), (16), and (17) are homogeneous in J^n and can give only the ratios of three components to one particular one, the remaining equation, Eq. (24), should give us the absolute values of J^n. We evaluate J^n in a special geodesic frame with $J^1=J^2=0$, and consequently

$$J^0=sJ^3 \quad (26)$$

with

$$s=\pm 1. \quad (27)$$

We get from Eqs. (11), (16), and (17)

$$T_{00}+2sT_{03}+T_{33}=0, \quad (28)$$

$$sT_{00;0}+2T_{03;0}+sT_{33;0}+T_{00;3}+2sT_{03;3}+T_{33;3}=0. \quad (29)$$

For the Einstein tensor to be equal to the energy-momentum tensor of a two-component spinor field, it must be possible to satisfy Eqs. (28) and (29) with Eq. (27) after a suitable rotation of the spacial axis of the coordinates. The last Eq. (24) is

$$J^3=s\frac{(sT_{10}+T_{13})^2T_{22}-2(sT_{10}+T_{13})(sT_{20}+T_{23})T_{12}+(sT_{20}+T_{23})^2T_{11}}{(sT_{20}+T_{23})(T_{00;1}+2sT_{03;1}+T_{33;1})-(sT_{10}+T_{13})(T_{00;2}+2sT_{03;2}+T_{33;2})}. \quad (30)$$

Since s was determined by Eqs. (28) and (29), we know J^3 and thus J^0 from Eq. (26). We reached a physical solution in a unique way, and we conclude that any other solution of Eq. (24) must give complex values for J^0 and J^3.

If $\sigma^{n\dot{\alpha}\beta}$ is known, we can find ψ_α from Eq. (10) up to an arbitrary phase function. But not any $\sigma^{n\dot{\alpha}\beta}$ which satisfies Eqs. (4) and (5) will be acceptable. If, for instance, $J^0<0$, we cannot have for $\sigma^{0\dot{\alpha}\beta}$ the unit matrix, because with this choice J^0 is necessarily positive or zero. We will have to choose for $\sigma^{0\dot{\alpha}\beta}$ the negative unit matrix and, in general, $\sigma^{0\dot{\alpha}\beta}$ may well change sign by going from one point of space-time to another point.

We note finally that Eq. (24) is invariant with respect to the substitution

$$T_{nm}{}^*=T_{nm}-(J_nB_m+J_mB_n), \quad (31)$$

where B_n is an arbitrary vector field. One obtains the same J^n for $T_{nm}{}^*$ as for T_{nm}.

4. WEYL EQUATIONS

The equations of the previous section hold independently of the field equations for the spinor field. We have mentioned already that

$$T=0 \quad (32)$$

is equivalent to one of these Weyl equations, and it is

easy to see that the conservation law, which follows from Eqs. (10) and (3),

$$J^{n}{}_{;n}=0, \tag{33}$$

is equivalent to another Weyl equation. If we had succeeded in solving Eq. (24) explicitly, we could have expressed Eq. (33) in terms of T_{nm}, or the Einstein tensor alone.

The last two equations do not exhaust the contents of Weyl's equations. The latter determine the time-development of the four quantities ψ_α, once they are known on a spacelike hypersurface. It would be desirable to have Weyl's equations expressed in terms of the current vector because such relations would supplement the algebraic equations (24), and would bring us nearer to the formulation of the necessary and sufficient conditions on T_{nm}. Although we have not been able to use the tensor formulation of Weyl's equations for this purpose, we will derive them here for the sake of completeness.

We use Eq. (12) to form $\epsilon_{nm}{}^{pq}J_{p;q}$ and make use of the anticommutation relation (4) and the definition (13) to obtain

$$\begin{aligned}\epsilon_{nm}{}^{pq}J_{p;q}=&i(-g)^{\frac{1}{2}}(U_{nm}-U_{mn})\\&-i\tfrac{1}{2}(-g)^{\frac{1}{2}}(\sigma_n{}^{\dot\alpha\beta}\sigma_{m\dot\alpha\nu}-\sigma_m{}^{\dot\alpha\beta}\sigma_{n\dot\alpha\nu})W^\nu\psi_\beta\\&+i\tfrac{1}{2}(-g)^{\frac{1}{2}}(\sigma_n{}^{\dot\mu\nu}\sigma_{m\dot\alpha\nu}-\sigma_m{}^{\dot\mu\nu}\sigma_{n\dot\alpha\nu})W^{\dot\alpha}\psi_{\dot\mu},\end{aligned} \tag{34}$$

where W^α and $W^{\dot\alpha}$ are supposed to vanish because of Weyl's equations. If $\psi_2=0$, $J^3>0$ and $J^0>0$, assuming that $\sigma^{3\dot\alpha\beta}$ is the usual z component of the Pauli matrices and $\sigma^{0\dot\alpha\beta}$ is the unit matrix. In such a frame only four of the six Eqs. (34) remain independent, and these allow us to calculate W^α and $W^{\dot\alpha}$ since the determinant is essentially $(\psi_1)^2(\psi_{\dot 1})^2$, and thus its vanishing would give a trivial state with no neutrinos present at all. We conclude then that the Eqs. (34) with $W^\alpha=W^{\dot\alpha}=0$ are equivalent to Weyl's equations

$$\epsilon_{nm}{}^{pq}J_{p;q}=i(-g)^{\frac{1}{2}}(U_{nm}-U_{mn}). \tag{35}$$

It remains to eliminate the tensor U_{nm} in terms of T_{nm} and J_n. To this purpose, we form

$$\epsilon_{nm}{}^{pq}J_{q;s}J_p=i(-g)^{\frac{1}{2}}(J_mU_{ns}-J_nU_{ms}) \tag{36}$$

and add expression (36) with n and s exchanged, and once again expression (36) with m and s exchanged

$$\begin{aligned}J_p(\epsilon_{nm}{}^{pq}J_{q;s}+\epsilon_{sm}{}^{pq}J_{q;n}+\epsilon_{ns}{}^{pq}J_{q;m})&\\=i(-g)^{\frac{1}{2}}(U_{nm}-U_{mn})J_s+(-g)^{\frac{1}{2}}&\\\times(J_mT_{ns}-J_nT_{ms}).&\end{aligned} \tag{37}$$

Insertion into (34) gives the desired, though not very simple, relation. Of special interest is the equation equivalent to (32):

$$\epsilon_{nm}{}^{pq}J_{p;q}J^m-(-g)^{\frac{1}{2}}T_{nm}J^m=-\tfrac{1}{2}(-g)^{\frac{1}{2}}TJ_n=0. \tag{38}$$

5. AFFINE SPIN CONNECTION

In this section we will examine the question of the determination of the spinor field by the current vector and afterwards, in the appendix, sketch the derivation of the conservation law for energy and momentum.

So far, covariant differentiation of spinors was not specifically defined and Infeld and van der Waerden's definition could have served as well as some other convention. We will now assume[9]

$$\gamma_{\alpha\beta;n}=0, \tag{39}$$

which results in a spinor analysis slightly different from Infeld and van der Waerden's, but is more convenient from our point of view. The definition of covariant differentiation is, of course, the standard one; for instance,

$$A^{\dot\alpha}{}_{\beta;n}=A^{\dot\alpha}{}_{\beta,n}+\Gamma^{\dot\alpha}{}_{\dot\mu n}A^{\dot\mu}{}_\beta-\Gamma^\nu{}_{\beta n}A^{\dot\alpha}{}_\nu, \tag{40}$$

and we assume also

$$\sigma^{n\dot\alpha\beta}{}_{;m}=0. \tag{41}$$

By writing (41) in full, multiplying it with $\sigma_{n\dot\lambda\lambda}\gamma_{\beta\mu}$, and subtracting an equivalent expression with λ and μ exchanged, we get, with the help of (39),

$$\begin{aligned}\Gamma^{\dot\alpha}{}_{\dot k m}=&-\tfrac{1}{4}(\sigma^{n\dot\alpha\beta}{}_{,m}+\{{}_{p}{}^{n}{}_{m}\}\sigma^{p\dot\alpha\beta})\sigma_{n\dot k\beta}\\&-\tfrac{1}{4}\delta^{\dot\alpha}{}_{\dot k}\gamma^{\lambda\mu}\gamma_{\lambda\mu,m}.\end{aligned} \tag{42}$$

We examine a special spinor transformation,

$$\gamma_{\alpha\beta}{}'=\gamma_{\alpha\beta}\exp(i\phi), \tag{43}$$

where ϕ is a real scalar function of the coordinates. Because of (7)

$$\gamma^{\alpha\beta'}=\gamma^{\alpha\beta}\exp(-i\phi), \tag{44}$$

and, by definition,

$$\gamma_{\dot\alpha\dot\beta}{}'=\gamma_{\dot\alpha\dot\beta}\exp(-i\phi). \tag{45}$$

The σ spinor-tensor is obviously invariant with respect to such phase transformations,[10] but the affine connection transforms according to

$$\Gamma^{\dot\alpha}{}_{\dot km}{}'=\Gamma^{\dot\alpha}{}_{\dot km}-i\tfrac{1}{2}\delta^{\dot\alpha}{}_{\dot k}\phi_{,m}, \tag{46}$$

and the spinor $\psi_{\dot\alpha}$ according to

$$\psi_{\dot\alpha}{}'=\psi_{\dot\alpha}\exp(-\tfrac{1}{2}i\phi). \tag{47}$$

Covariant differentiation of a spinor was defined so as to make $\psi_{\dot\alpha;n}$ a spinor-tensor of the indicated rank and a phase transformation implies, therefore,

$$\psi_{\dot\alpha;n}{}'=\psi_{\dot\alpha;n}\exp(-\tfrac{1}{2}i\phi). \tag{48}$$

[9] W. L. Bade and H. Jehle, Revs. Modern Phys. 25, 714 (1953).

[10] A more general formalism with a recommendable distinction between phase and gauge invariance has been given by H. A. Buchdahl, Quart. J. Math. (Oxford) 9, 109 (1958), but the above formulation is quite sufficient for our purpose and the phrase "phase transformation" will be used only in the restricted sense.

We assume now that $\sigma^{n\dot{\alpha}\beta}$ and g_{nm} are given, and that some $\gamma_{\alpha\beta}$, which satisfies Eqs. (4) and (5), is also known. Any other $\gamma_{\alpha\beta}'$ connected with $\gamma_{\alpha\beta}$ by (43) could be used as well, but we will fix our attention at one arbitrarily choosen $\gamma_{\alpha\beta}$ and calculate the corresponding affine spin connection $\Gamma^{\alpha}{}_{\beta n}$ from (42). The tensor formulation of the theory allows us to calculate the spinor field everywhere up to an arbitrary space-time dependent phase factor. Although we also know the ordinary differential quotients of the spinor variables, we do not know yet the covariant differential quotients, because the chosen $\gamma_{\alpha\beta}$ and the calculated $\psi_\alpha{}^*$ may not be—and will not be except by a peculiar coincidence—in the same phase frame. We still have to find the ψ_α, which belongs to the same phase frame as the choosen $\gamma_{\alpha\beta}$,

$$\psi_{\dot{\alpha}}=\psi_{\dot{\alpha}}{}^* \exp(-\tfrac{1}{2}i\varphi) \tag{49}$$

and

$$\psi_{\dot{\alpha};n}=(\psi_{\dot{\alpha};n}{}^*-\tfrac{1}{2}i\psi_{\dot{\alpha}}{}^*\varphi_{;n}) \exp(-\tfrac{1}{2}i\varphi), \tag{50}$$

where the semicolon stands here, as before, for the covariant differentiation (40) formed with the $\Gamma^{\dot{\alpha}}{}_{\dot{\beta}n}$ from the chosen $\gamma_{\alpha\beta}$. We see that expression (2) calculated for the $\psi_\alpha{}^*$ will not be equal to the given tensor T_{nm}. In fact,

$$T_{nm}=T_{nm}{}^*+(J_n\varphi_{,m}+J_m\varphi_{,n}), \tag{51}$$

where $T_{nm}{}^*$ is expression (2) formed with $\psi_{\dot{\alpha}}{}^*$ and $\psi_{\alpha;n}{}^*$.

The appearance of the unknown phase function has been anticipated at the beginning of the third section. We stated there that the $J^n{}_{,m}$ in a geodesic frame does not determine $\psi_{\alpha,n}$, but that the still unknown gradient of the phase function at the point of reference can be found from four components of the energy-momentum tensor. With the help of the current vector, we have found $\psi_{\alpha,n}{}^*$, but this is not yet the final result and we again have to use the given energy-momentum tensor in Eq. (51) to complete the solution.

Another way of explaining the same difficulty is by recalling that the specific form of the covariant differential quotients was irrelevant for our considerations in Secs. 3 and 4, and we could have implied all the time the more general formula,

$$\psi_{\alpha;n}=\psi_{\alpha,n}-\Gamma^{\beta}{}_{\alpha n}\psi_\beta-\tfrac{1}{2}iB_n\psi_\alpha \tag{52}$$

with B_n an arbitrary vector field.[11] The current vector gives no information about B_n and some $\psi_\alpha{}^*$, which satisfies Eq. (10), need not give T_{nm} when inserted in the expression (2). An equation just like (51) will have to be solved to determine B_n.

[11] See Buchdahl, footnote 10. The wave equation $\Box\psi_\alpha=0$ in a geodesic frame is obtained only if B_n is the gradient of a scalar. The expression (42) for $\Gamma^{\alpha}{}_{\beta n}$ may still hold because it rests on Eqs. (39) and (40), if the semicolon stands there for covariant differentiation without the B_n term. Besides phase transformations as spinor transformations we could envisage phase transformations performed only on $B_n'=B_n+\varphi_{,n}$ and $\psi_{\dot{\alpha}}'=\psi_{\dot{\alpha}}\exp(-\frac{1}{2}i\varphi)$, but not on $\gamma_{\alpha\beta}$.

The invariance property (31) is not true for (35) with (37). This explains why we do not need to solve additionally to (51) the set of equations,

$$W^\alpha=(W^{\alpha*}-\tfrac{1}{2}i\sigma^{n\dot{\beta}\alpha}\psi_{\dot{\beta}}{}^*\varphi_{,n}) \exp(-\tfrac{1}{2}i\varphi)=0, \tag{53}$$

although the $\psi_\alpha{}^*$ will not satisfy Weyl's equations. But Eq. (35) is a consequence of $W^\alpha=0$ rather than of $W^{\alpha*}=0$, and already takes into account the vanishing of the bracket in Eq. (53). Moreover, Eqs. (35) and (37) should be viewed as relations between T_{nm} and its derivatives, which could be written down if only we knew the algebraic solutions J^n of Eq. (24).[12]

Our task would be to show the uniqueness of the solution φ of (51) up to an arbitrary constant, and exhibit the integrability conditions. This can be carried out only to a rather limited extent as long as we do not know J^n as function of T_{nm} and, more important, $T_{nm}{}^*$ as a function of J^n, and thus of T_{nm}. The implication of (51) that the matrix $T_{nm}-T_{nm}{}^*$ can have at most the rank two is, of course, already contained in our statement that $\psi_\alpha{}^*$, which was obtained from J^n, can differ from the correct ψ_α at most in the phase factor. The easily derived consequence of (51),

$$(T_{nm}-T_{nm}{}^*)J^m=-\tfrac{1}{2}T^*J_n, \tag{54}$$

where T^* is the trace of $T_{nm}{}^*$, is also contained in a previous statement; the first part of Eq. (38) will hold also for $T_{nm}{}^*$ and T^*, and J^n and $J^n{}_{;m}$ are the same, whether formed with ψ_α or with $\psi_\alpha{}^*$

$$\epsilon_{nm}{}^{pq}J_{p;q}J^m=(-g)^{\frac{1}{2}}(T_{nm}{}^*-\tfrac{1}{2}T^*g_{nm})J^m. \tag{55}$$

By subtracting Eq. (38), we regain (54) without having used (51).

6. CONCLUSIONS

The studies presented in this paper may be divided into three parts. The first part, which culminates in the four algebraic equations (24) for the current vector, is of interest even apart from Rainich's problem. We have shown the contents of these equations by introducing a special coordinate frame in terms of the current vector. Although the results of this procedure are conclusive, it would be desirable, and it is essential for the Rainich formulation of the theory, to solve these equations in a covariant form and this may well be possible with the help of more sophisticated methods. The second part of the paper was devoted to a study of Weyl's equations expressed in the current vector. Although we have found such expressions, some of them are obviously redundant. The final form (35) with (37) contains 24 equations of which only 4 can be relevant. It would be desirable to find a more economical way of writing Weyl's equations in tensor form, without

[12] It would seem possible to replace Eq. (51) by Eq. (53) to find the correct phase, but we have not analyzed the steps to justify this attitude.

introducing new variables since the main point in favor of our method consists in operating with physically meaningful tensors and this feature is worth preserving. The third part of the paper deals with the calculation of the spinors themselves. Apart from a mathematical incompleteness of our studies, the attitude of taking $\sigma^{n\dot{\alpha}\beta}$ as a given quantity, subject to the Eqs. (4) and (5), is unsatisfactory because the original choice may turn out to be unacceptable. Since $\sigma^{n\dot{\alpha}\beta}$ cannot be measured, one ought to show how to derive it. The connection between spin-curvature tensor and Riemann tensor would be important for this problem.

The necessary and sufficient conditions for T_{nm} which we were unable to write down would provide us also with the answer to our question for a phenomenological Einstein theory in which neither the spinor field nor the derived tensors like the current vector enter. We would substitute for T_{nm} the expression on the left-hand side of Eq. (9) and so obtain the required relations. Of course $T_{nm}=0$ will be one trivial solution corresponding to the usual Einstein equations in the absence of a neutrino field. But the general equations are, in any case, too complicated to be of any use.

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APPENDIX

We recall here the derivation of

$$T^{n}{}_{m;n}=0 \tag{A.1}$$

corresponding to the contracted Bianchi identity of the Einstein tensor. With (2) we obtain for (A.1),

$$\sigma^{n\dot{\alpha}\beta}(\psi_{\dot{\alpha};mn}\psi_{\beta}-\psi_{\dot{\alpha}}\psi_{\beta;mn}) +\sigma_{m}{}^{\dot{\alpha}\beta}(\psi_{\beta}\Box\psi_{\dot{\alpha}}-\psi_{\dot{\alpha}}\Box\psi_{\beta})=0, \tag{A.2}$$

where $\Box$ stands for the covariant d'Alembert operator. By definition,

$$\psi_{\beta;mn}=\psi_{\beta;nm}+P^{\alpha}{}_{\beta mn}, \tag{A.3}$$

where $P^{\alpha}{}_{\beta mn}$ is the curvature spinor,

$$P^{\alpha}{}_{\beta mn}=-\Gamma^{\alpha}{}_{\beta m,n}+\Gamma^{\alpha}{}_{\beta n,m}+\Gamma^{\mu}{}_{\beta n}\Gamma^{\alpha}{}_{\mu m}-\Gamma^{\mu}{}_{\beta m}\Gamma^{\alpha}{}_{\mu n}. \tag{A.4}$$

We find

$$\sigma^{n\dot{\alpha}\beta}{}_{;pq}-\sigma^{n\dot{\alpha}\beta}{}_{;qp}=\sigma^{m\dot{\alpha}\beta}R^{n}{}_{mqp}+\sigma^{n\dot{\mu}\beta}P^{\dot{\alpha}}{}_{\dot{\mu}qp} +\sigma^{n\dot{\alpha}\nu}P^{\beta}{}_{\nu qp}=0 \tag{A.5}$$

and

$$P^{\beta}{}_{\alpha qp}=-\tfrac{1}{4}\sigma_{n\dot{\iota}\alpha}\sigma^{m\dot{\iota}\beta}R^{n}{}_{mqp} \tag{A.6}$$

since $P^{\alpha}{}_{\alpha qp}=0$. Insertion into the first term of (A.2) leads, after some manipulations and use of (12), to

$$\tfrac{1}{2}i(-g)^{-\frac{1}{2}}\epsilon^{rnpq}J_{r}R_{mnqp}, \tag{A.7}$$

and this vanishes because of the cyclic symmetry of the Riemann tensor. To show that the second bracket in (A.2) vanishes, we derive the iterated Weyl equations. Applying $\sigma^{m}{}_{\dot{\alpha}\kappa}\partial/\partial x^{m}$ on (3) and again using (A.3) and (A.5)

$$\Box\psi_{\mu}+\tfrac{1}{8}\sigma^{m\dot{\alpha}\beta}\sigma^{n}{}_{\dot{\alpha}\kappa}\sigma_{q\dot{\lambda}\beta}\sigma^{p\dot{\lambda}\mu}R^{q}{}_{pnm}\psi_{\mu}=0. \tag{A.8}$$

Repeated application of the anticommutation relation gives

$$\sigma^{m\dot{\alpha}\beta}\sigma_{q\dot{\lambda}\beta}\sigma^{p\dot{\lambda}\mu}R^{q}{}_{pnm}=2\sigma^{p\dot{\alpha}\mu}R_{pn}, \tag{A.9}$$

and thus

$$\Box\psi_{\kappa}+\tfrac{1}{4}R\psi_{\kappa}=0, \tag{A.10}$$

which completes the proof of (A.1).

Linearized Plasma Oscillations in Arbitrary Electron Velocity Distributions*

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This paper is a mathematical examination of the linearized small disturbances in the steady distribution $f_0(\mathbf{q})$ of the velocities $\mathbf{q}$ of the electrons in an electrostatic, collisionless plasma with motionless protons. It is assumed that $g_0(u)=\iint f_0(u,v,w)dvdw$ has an integrable derivative with respect to u for all axis orientations. An existence and uniqueness theorem for the initial value problem is given, and it is shown that no disturbance can grow faster than $\exp\omega_p t$, where ω_p is the electron plasma frequency. Consequently, one can base a stability theory on Laplace transforms with respect to time, as Landau has done. The limits of validity of Landau's stability criterion are explored: that $g_0(u)$ is stable if there are no wave numbers k for which $\mathcal{L}(s)=k^2\omega_p^{-2}-\int_{-\infty}^{\infty} g_0'(u)(u-s)^{-1}du$ has zeros in the upper complex s half-plane. To ensure instability, the zeros must have positive imaginary parts or a multiplicity of 2 or greater. To insure stability, the initial disturbance must be not only integrable, but square integrable with respect to u. The Maxwell distribution is unstable to certain integrable disturbances. All isotropic, three-dimensional distributions $f_0(\mathbf{q})=h(q^2)$ for which $x^{\frac{1}{2}}h(x)$ is absolutely continuous and square integrable, and $h(x)+2xh'(x)$ is bounded, are stable to integrable, square integrable disturbances. This explains Van Kampen's ability to solve the initial value problem by superposing normal modes (solutions with complex, exponential time dependence) with real frequencies; he implicitly introduced stability by considering only isotropic distributions $f_0(\mathbf{q})$. His method is extended to unstable f_0 as a technique independent of Landau's for solving the initial value problem. If f_0 is unstable, the normal modes are not complete, and a normal mode analysis can lead to erroneous positive conclusions about stability. Finally, the linear theory predicts that in stable plasmas the neglected term will grow linearly with time at a rate proportional to the initial disturbance amplitude, destroying the validity of the linear theory, and vitiating positive conclusions about stability based on it. In a thermonuclear plasma with $T=10^8$ °K and $N=10^{15}$ electrons/cm^3, a disturbance of wavelength 1 cm and initial amplitude 1 v can no longer be treated by the linear theory after 220 μsec.

I. INTRODUCTION

THE present paper is devoted to a mathematical examination of two schemes, Landau's[1] and Van Kampen's,[2] which have been proposed for finding the time dependence of the electrons' Boltzmann distribution function in a nearly neutral, nearly steady, nearly homogeneous plasma of infinite extent in which the effects of short-range collisions, magnetic fields, and the motions of the protons are neglected. With these approximations, the electrons' motion is entirely determined by the average electrostatic field they set up, and their Boltzmann equation is linearized. The mathematical problem is then to determine from its initial form the time dependence of the small perturbation in the electrons' Boltzmann distribution function, given the form of the steady, homogeneous, neutral electron distribution which is being perturbed. Since collisions are neglected, this steady distribution can have any velocity dependence as long as it is independent of position and provides enough electrons for electrical neutrality when combined with the background of motionless protons.

Van Kampen's approach to the linearized problem consists in finding the normal modes of the linearized Boltzmann equation (those solutions whose time dependence is sinusoidal) and writing the initial perturbation as a superposition of normal modes. Van Kampen never explicitly restricts himself to stable plasmas, and yet his results are false for unstable ones. We will show where he has limited his theory to stable plasmas and how to modify it so as to apply to unstable ones. It turns out that for an unstable plasma, the real and complex exponentially time-dependent solutions do not always form a complete set, and as a result all the disturbances with such time dependence may be bounded while other disturbances grow with time.

Because of this situation, Landau's Laplace transformation of the linearized Boltzmann equation with respect to time seems the simpler way to approach the problem, and we will follow Landau in most of the present paper. We propose to study four questions besides Van Kampen's normal mode approach.

First, in Secs. III and IV we prove an existence and uniqueness theorem for the linearized initial value problem. This is necessary because *a priori* that problem might have solutions which grow too rapidly to have Laplace transforms in time; such pathological solutions would be missed in a stability analysis based on Laplace transforms. We succeed in proving that all disturbances grow at rates slower than the plasma frequency, and hence do have Laplace transforms.

Second, in Sec. V we examine in detail Landau's criterion for the stability of a neutral plasma. It turns out that the results depend heavily on the smoothness of the initial disturbances which are allowed.

Third, in Sec. VI we apply Landau's criterion to several examples. In particular, we show that any isotropic, steady, homogeneous electron velocity distribution is stable. Van Kampen's restriction of his discussion to such distributions means that his arguments must be reconsidered for unstable distributions. This reconsideration occupies Sec. VII.

Fourth, in Sec. VIII we show that the neglected nonlinear terms in the Boltzmann equation grow linearly with time at a rate proportional to their initial ampli-

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[1] L. Landau, J. Phys. (U.S.S.R.) **10**, 25 (1946).
[2] N. G. Van Kampen, Physica **21**, 949 (1955).

tude. In a typical thermonuclear plasma, an initial disturbance which produces a potential of 1 v will have changed in such a way as to vitiate the linear theory in a time of the order of msec.

The problem under discussion is physically simple and mathematically intricate, but not difficult in principle. The justification for treating it in the present detail is that it is the simplest example of a large class of plasma problems in which collisions are neglected and the Boltzmann equation is linearized. In the present instance, the mathematical consequences of these approximations can be discussed in detail.

II. BASIC EQUATIONS

Let the number N of positive ions per unit volume be independent of time and position. Let $Nf(\mathbf{r},\mathbf{q},t)$ be the number of electrons per unit volume of velocity space and per unit volume of real space which have position $\mathbf{r}$ and velocity $\mathbf{q}$ at time t. Assume that $f(\mathbf{r},\mathbf{q},t)=f_0(\mathbf{q})+f_1(\mathbf{r},\mathbf{q},t)$, where $f_1 \ll f_0$ and $f_0(\mathbf{q})\geq 0$, and, to ensure electrical neutrality of the undisturbed plasma,

$$\int f_0(\mathbf{q})d\mathbf{q}=1. \tag{1}$$

In neglecting short-range collisions and magnetic fields, the Boltzmann equation for f is

$$\frac{\partial f}{\partial t}+\mathbf{q}\cdot\frac{\partial f}{\partial \mathbf{r}}-\frac{e}{m}\mathbf{E}\cdot\frac{\partial f}{\partial \mathbf{q}}=0, \tag{2}$$

where e and m are the electronic charge and mass, and the electrostatic field $\mathbf{E}$ is given exactly by

$$\mathbf{E}(\mathbf{r},t)=-eN\int\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}d\mathbf{r}'\int f_1(\mathbf{r}',\mathbf{q}',t)d\mathbf{q}'. \tag{3}$$

If products of terms of the order of f_1 are neglected, (2) becomes

$$\frac{\partial f_1}{\partial t}+\mathbf{q}\cdot\frac{\partial f_1}{\partial \mathbf{r}}-\frac{e}{m}\mathbf{E}\cdot\frac{\partial f_0}{\partial \mathbf{q}}=0. \tag{4}$$

Now let $f_1(k,q,t)$ be the Fourier transform of $f_1(\mathbf{r},\mathbf{q},t)$ with respect to $\mathbf{r}$

$$f_1(\mathbf{k},\mathbf{q},t)=\int f_1(\mathbf{r},\mathbf{q},t)e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}.$$

The problem is to find $f_1(\mathbf{k},\mathbf{q},t)$ given $f_1(\mathbf{k},\mathbf{q},0)$. Since conservation of total charge in all space implies that f_1 vanishes at all times for $\mathbf{k}=\mathbf{0}$, and hence is known, it will be assumed henceforth that $\mathbf{k}\neq\mathbf{0}$.

If the Fourier transform of $\mathbf{E}$ is eliminated from the Fourier transforms of Eqs. (3) and (4), a single equation for f_1 is obtained:

$$\left(\frac{1}{i}\frac{\partial}{\partial t}+\mathbf{k}\cdot\mathbf{q}\right)f_1(\mathbf{k},\mathbf{q},t)=\frac{\omega_p^2}{k^2}\left(\mathbf{k}\cdot\frac{\partial f_0}{\partial \mathbf{q}}\right)\int f_1(\mathbf{k},\mathbf{q}',t)d\mathbf{q}'. \tag{5}$$

Here $\omega_p=(4\pi e^2N/m)^{\frac{1}{2}}$ is the electron plasma frequency.

Now fix $\mathbf{k}$ and choose the x axis parallel to $\mathbf{k}$. Let u, v, w be the x, y, z components of $\mathbf{q}$. Then Eq. (5) becomes

$$\left(\frac{1}{ik}\frac{\partial}{\partial t}+u\right)f_1(u,v,w,t)=v_p^2\frac{\partial f_0}{\partial u}\int f_1(u',v',w',t)du'dv'dw', \tag{6}$$

where $v_p=\omega_p/k$ and the dependence of f_1 on $\mathbf{k}$ is no longer explicitly shown. If the integral on the right were a known function of time, (6) would immediately give $f_1(u,v,w,t)$ in terms of $f_1(u,v,w,0)$. Therefore, to solve (6), it is sufficient to find

$$g_1(u,t)=\int f_1(u,v,w,t)dvdw \tag{7}$$

as a function of u and t (and $\mathbf{k}$). For this purpose, integrate (6) with respect to v and w. The result is

$$\left(\frac{1}{ik}\frac{\partial}{\partial t}+u\right)g_1(u,t)=v_p^2\frac{dg_0(u)}{du}\int_{-\infty}^{\infty}g_1(u',t)du', \tag{8}$$

where

$$g_0(u)=\int f_0(u,v,w)dudw.$$

It is the purpose of the present paper to discuss in detail the initial value problem for Eq. (8). That equation is formally equivalent to (3) and (4), but the author has not examined whether there are solutions of (3) and (4), which do not have Fourier transforms with respect to $\mathbf{r}$, and yet are in some sense physically meaningful. Therefore the discussion is applicable only to solutions of (3) and (4) which can be Fourier transformed. This class of solutions includes all those for which $\int\int|f_1(r,q,t)|drdq$ is finite.

It should be pointed out that Eq. (8) is applicable also to small disturbances in a homogeneous, collisionless plasma containing a uniform, externally imposed magnetic field, if the disturbance f_1 involves only motions parallel to the magnetic field and the undisturbed state $f_0(\mathbf{q})$ is symmetric under rotations about the direction of that field.

III. UNIQUENESS THEOREM AND A BOUND ON THE GROWTH RATE

If we follow Landau,[1] we shall deduce most of the properties of the solution $g_1(u,t)$ of (8) by examining its Laplace transform with respect to time. But if (8) has solutions which grow too rapidly to have Laplace transforms, then no results deduced from the existence of a Laplace transform will apply to these exceptional solutions. In particular, a stability criterion for $g_0(u)$ based on Laplace transform techniques may predict that

$g_0(u)$ is stable simply because all perturbations g_1, which grow at all, grow too rapidly to have Laplace transforms.

It might be felt that (8), being linear, would have no solutions without Laplace transforms. As a counter example, $(T-t)^{-\frac{1}{2}}\exp(x^2/T-t)$ is a solution of the linear equation $4(\partial f/\partial t)+(\partial^2 f/\partial x^2)=0$, if $-\infty<x<\infty$ and $0\leq t<T$.

To remove this difficulty, we show that any solution $g_1(u,t)$ of (8) in an interval $0\leq t<T$ is uniquely determined by its initial form $g_1(u,0)$; then, in the following section, we show that for any $g_1(u,0)$, (8) does have a solution $g_1(u,t)$ in $0\leq t<\infty$ which takes the given initial form and which has a Laplace transform with respect to time. Thus every solution of (8) on a finite interval $0\leq t<T$ agrees with a solution on $0\leq t<\infty$ which has a Laplace transform.

We assume throughout the present paper that $|g_0'(u)|$ is integrable on $-\infty<u<\infty$. With slight modifications of statement, the results of the paper remain true if this condition is replaced by the weaker one that $g_0(u)$ be of bounded variation on $-\infty<u<\infty$, but we do not propose to discuss these modifications.

We also assume that if a solution $g_1(u,t)$ of (8) is to be physically realizable during an interval $0\leq t<T$, then the integral

$$Q(t)=\int_{-\infty}^{\infty} g_1(u,t)du \tag{10}$$

for the charge density at the given wave number $\mathbf{k}$ must be independent of the order in which the electrons are counted, so that

$$A(t)=\int_{-\infty}^{\infty}|g_1(u,t)|du<\infty, \tag{11}$$

if $0\leq t<T$. We contemplate the possibility *a priori* that $A(t)$ or $Q(t)\to\infty$ as $t\to T$, but we do not consider a solution of (8) to be physically realizable, or even mathematically meaningful, unless there is some interval $0\leq t<T$ in which $Q(t)$ is finite, so that

$$\int_0^t|Q(\tau)|d\tau<\infty, \tag{12}$$

if $0\leq t<T$. In the rest of this paper, no function $g_1(u,t)$ will be considered to be a "solution" of (8), unless there is some finite interval $0\leq t<T$ in which it satisfies (11) and (12).

Equation (8) would seem to force us to demand also that $\partial g_1/\partial t$ exist, but this demand can be avoided if we replace (8) by the equivalent integral equation:

$$g_1(u,t)=g_1(u,0)e^{-iku t}+ikv_p{}^2g_0'(u)\times\int_0^t Q(\tau)e^{iku(\tau-t)}d\tau. \tag{13}$$

From (11), (12), and (13) we now propose to show that if $0\leq t<T$ then

$$|Q(t)|\leq A(0)\cosh\omega_p t; \tag{14}$$

and that at every u for which $g_1(u,0)$ and $g_0'(u)$ are defined, and hence at almost every u,

$$|g_1(u,t)|\leq|g_1(u,0)|+A(0)v_p|g_0'(u)|\sinh\omega_p t. \tag{15}$$

To prove (14), we integrate (13) with respect to u, and use Fubini's theorem to justify the inversion of the order of integration in the double integral on the right. After an integration by parts with respect to u and to t, the result is

$$Q(t)=\int_{-\infty}^{\infty}g_1(u,0)e^{-iku t}du-\omega_p{}^2\int_0^t d\tau_2 Q(\tau_2)\int_{-\infty}^{\infty}dug_0(u)e^{iku(\tau_2-t)}. \tag{16}$$

Since $g_0(u)\geq 0$ and $\int g_0(u)du=1$, it follows that

$$|Q(t)|<A(0)+\omega_p{}^2\int_0^t d\tau_1\int_0^{\tau_1}d\tau_2|Q(\tau_2)|. \tag{17}$$

Denote the double integral on the right of (17) by $F(t)$. Then if $h(t)=F''(t)-\omega_p{}^2F(t)$, $|h(t)|\leq A(0)$ and

$$F(t)=\int_0^t d\tau_1\int_0^{\tau_1}d\tau_2 h(\tau_2)e^{\omega_p(2\tau_1-\tau_2-t)},$$

so $0\leq F(t)\leq A(0)\omega_p{}^{-2}[\cosh(\omega_p t)-1]$. The substitution of this upper bound for the double integral into (17) gives (14). The substitution of (14) into the obvious inequality obtained from (13) gives (15).

Now we note that because $g_1(u,0)$ and $g_0(u)$ are integrable with respect to u, (12) and (16) imply that $Q(t)$ depends continuously on t in $0\leq t<T$. But then (13) implies that for every u at which $g_1(u,0)$ and $g_0'(u)$ are defined, $\partial g_1(u,t)/\partial t$ exists and is continuous as a function of t in $0\leq t<T$, and can be computed by differentiating (13). Thus $g_1(u,t)$ satisfies (8) in $0\leq t<T$ for every u at which $g_1(u,0)$ and $g_0'(u)$ are defined. (We note in passing that if $\int|ug_1(u,0)|du<\infty$, then from (16) and the Lebesque bounded convergence theorem dQ/dt exists and is continuous. In general, if $g_1(u,0)$ has n finite moments, $Q(t)$ and $\partial g_1/\partial t$ have n continuous time derivatives.)

A second consequence of inequalities (14) and (15) is that if $A(0)=0$, $g_1(u,t)=0$. But since (13) is linear, it follows that any function $g_1(u,t)$ which satisfies (11), (12), and (13) in $0\leq t<T$ is uniquely determined in that interval by its initial form, $g_1(u,0)$.

A third consequence of inequalities (14) and (15) is that no disturbance $g_1(u,t)$ can grow at a rate faster than ω_p. Thus the only way in which a solution $g_1(u,t)$ of (11), (12), (13) can fail to have a Laplace transform is that for some reason it cannot be extended outside $0\leq t<T$

as a valid solution of those equations. The next section will eliminate this possibility.

IV. AN EXISTENCE THEOREM AND AN EXPLICIT SOLUTION

In this section we show that if $g_0'(u)$ is integrable and $g(u)$ is any integrable function of u, then there is a function $g_1(u,t)$ which satisfies (11), (12), and (13) if $0 \leq t < \infty$, and for which $g_1(u,0) = g(u)$. Having shown so much, we can conclude from (14) and (15) that $Q(t)$ and $g_1(u,t)$ have Laplace transforms with respect to t.

At the outset we follow Landau[1] and proceed purely formally. We introduce the Laplace transform of $g_1(u,t)$,

$$\gamma(u,s) = \int_{-\infty}^{\infty} e^{ikst} g_1(u,t)\,dt.$$

In terms of our variable s, the usual Laplace transform variable p is $-iks$, so the right complex p half-plane corresponds to the upper s half-plane if $k>0$. Then, still proceeding formally, Eq. (8) becomes, for positive k,

$$\gamma(u,s) = \frac{g_1(u,0)}{ik(u-s)} = v_p^2 \frac{g_0'(u)}{u-s} \int_{-\infty}^{\infty} \gamma(v,s)\,dv. \tag{18}$$

Now we introduce the functional operator $\mathfrak{K}_{su}$ defined by

$$\mathfrak{K}_{su} f(u) = \int_{-\infty}^{\infty} \frac{f(u)}{u-s}\,ds, \tag{19}$$

where u is real and s is in the open complex upper half-plane. If we integrate (18) with respect to u, we find

$$\int_{-\infty}^{\infty} \gamma(u,s)\,du = \frac{\mathfrak{K}_{su} g_1(u,0)}{ikv_p^2 \mathfrak{L}(s)}, \tag{20}$$

where

$$\mathfrak{L}(s) = \frac{1}{v_p^2} - \mathfrak{K}_{su} g_0'(u) = \frac{1}{v_p^2} - \int_{-\infty}^{\infty} \frac{g_0(u)}{(u-s)^2}\,du. \tag{21}$$

Hence, from (18)

$$ik\gamma(u,s) = \frac{g_1(u,0)}{u-s} + \frac{g_0'(u)}{u-s}\left(\frac{\mathfrak{K}_{sv} g_1(v,0)}{\mathfrak{L}(s)}\right). \tag{22}$$

Still proceeding formally, we use the complex inversion formula for the Laplace transform to find $g_1(u,t)$ from $\gamma(u,s)$ as given in (22):

$$g_1(u,t) = g_1(u,0)e^{-iku t} + \frac{g_0'(u)}{2\pi i} \times \int_{-\infty+ib}^{\infty+ib} \frac{e^{-ikst}\mathfrak{K}_{sv} g_1(v,0)}{(u-s)\mathfrak{L}(s)}\,ds, \tag{23}$$

where b is a positive real number larger than the (unspecified) abscissa of absolute convergence of $\gamma(u,s)$, and $k>0$.

Now we propose to show that (23) has more than formal content. Specifically, if $b > v_p$ and $g_1(u,0)$ are replaced by $g(u)$ at every occurrence on the right side of (23), then we can show that the integral in (23) converges so that (23) defines a function $g_1(u,t)$. We can further show that this $g_1(u,t)$ satisfies (11), (12), and (13), if in (13) $g_1(u,0)$ is replaced by $g(u)$, so that $g_1(u,0) = g(u)$.

The basis for the whole argument is an analysis of the functional operator $\mathfrak{K}_{su}$. We need a number of facts about this operator which we collect here as lemmas.

If $s = x+iy$ is a complex number, let $\Re s = x$ and $\Im s = y$. If $f(u)$ is a function of the real variable u, define

$$\|f(u)\|_n = \left[\int_{-\infty}^{\infty} |f(u)|^n du\right]^{1/n},$$

where n is a positive integer. If $f(s)$ is a function of the complex variable s, define

$$\|f(s)\|_{bn} = \left[\int_{-\infty}^{\infty} |f(x+ib)|^n dx\right]^{1/n},$$

where n is a positive integer and x and b are real.

Lemma 1: If $f(u)$ is integrable or square integrable, $\mathfrak{K}_{su} f(u)$ is analytic in the open upper s half-plane.

This lemma follows immediately from the Lebesque bounded convergence theorem.

Lemma 2: Suppose that b is a positive number and $\|f(u)\|_1$ is finite. Then

$$\int_{-\infty+ib}^{\infty+ib} \left|\frac{\mathfrak{K}_{su} f(u)}{v-s}\right| ds < \frac{\pi}{b}\|f(u)\|_1$$

for every real v.

To prove lemma 2, it suffices to prove that if u and v are real,

$$\int_{-\infty+ib}^{\infty+ib} ds \int_{-\infty}^{\infty} du \left(\frac{|f(u)|}{|u-s|\,|v-s|}\right) \leq \frac{\pi}{b} f_1.$$

But if this inequality can be proved in either order of integration, Fubini's theorem proves it for the other order. Hence it suffices to prove $K(u,v) < \pi b^{-1}$, where

$$K(u,v) = \int_{-\infty+ib}^{\infty+ib} \frac{ds}{|u-s|\,|v-s|};$$

But by Schwarz's inequality, $K(u,v)^2 \leq K(u,u)K(v,v)$ and clearly $K(u,u) = K(v,v) = \pi b^{-1}$.

Lemma 3: Let α be a positive number less than v_p^{-2} and write the complex number s as $x+iy$. Let $C_1(\alpha)$ and $C_2(\alpha)$ be the two regions of the upper s half-plane defined by the following inequalities:

$$C_1(\alpha): \quad y^2 > (v_p^{-2} - \alpha)^{-1}.$$

$$C_2(\alpha): \quad \text{if} \quad \sigma = \pm 1, \quad \sigma x > 2v_p$$

and also

$$y^2 > [v_p^{-2} - \alpha - 4x^{-2}]^{-1} \int_{\sigma x/2}^{\infty} g_0(\sigma u)\,du.$$

Then if s is in $C_1(\alpha)$ or $C_2(\alpha)$, $|\mathcal{L}(s)| > \alpha$.

First suppose s is in $C_1(\alpha)$. Then $|u-s|^{-2} \leq v_p^{-2} - \alpha$ for real u, and the lemma follows immediately from (21), since $g_0(u) \geq 0$ and $\int g_0(u)\,du = 1$. Next suppose s is in the right half of $C_2(\alpha)$, where $\sigma = +1$. Then

$$\frac{1}{v_p^2} - \mathcal{L}(s) = \int_{-\infty}^{x/2} \frac{g_0(u)\,du}{(u-x-iy)^2} + \int_{x/2}^{\infty} \frac{g_0(u)\,du}{(u-x-iy)^2}.$$

Since $|u-x-iy|^{-2} \leq 4x^{-2}$ in the first integral and $\leq y^{-2}$ in the second, the inequalities defining $C_2(\alpha)$ imply $|\mathcal{L}(s)| > \alpha$. The left half of $C_2(\alpha)$ is treated similarly.

We point out some immediate consequences of lemma 3. If α and b are any positive numbers, the set of complex s's for which $\Im s \geq b$, and which lie neither in $C_1(\alpha)$ nor $C_2(\alpha)$ is closed and bounded. But all the zeros of $\mathcal{L}(s)$ for which $\Im s \geq b$ must lie in this set. Since $\mathcal{L}(s)$ is analytic in the open upper half-plane, it follows that $\mathcal{L}(s)$ has only finitely many zeros for which $\Im s \geq b$, and none for which $\Im s > v_p$. It follows further that if $b > v_p$ then on the line $\Im s = b$, $|\mathcal{L}(s)| \geq v_p^{-2} - b^{-2}$.

Now we return to formula (23), in which we take $b > v_p$ and on the right replace $g_1(u,0)$ everywhere by the given integrable function $g(u)$. Then by lemmas 2 and 3, the integrand on the right in (23) is an integrable function of s along the line $\Im s = b$, and the integral is not larger in absolute value than $(v_p^{-2} - b^{-2})^{-1} \pi b^{-1} \|g(u)\|_1 e^{kbt}$. Since $g(u)$ and $g_0'(u)$ are integrable, it follows that the function $g_1(u,t)$ defined by (23) does satisfy (11) and (12) for all t, depends continuously on t, and for each u at which $g(u)$ and $g_0'(u)$ are defined, has a Laplace transform with respect to t. By the complex inversion theorem, this Laplace transform is the $\gamma(u,s)$ of (22) if $g_1(u,0)$ is replaced by $g(u)$ everywhere on the right in (22). But if $\Im s \geq b$, the integral

$$\int_{-\infty}^{\infty} du \int_0^{\infty} dt e^{iks t} g_1(u,t)$$

converges absolutely, and hence can be integrated in either order. Thus, if $Q(t)$ is defined by (10) in terms of the $g_1(u,t)$ defined by (23), the Laplace transform of $Q(t)$ is $\int \gamma(u,s)du$, and is given correctly by (20), $g_1(u,0)$ being replaced by $g(u)$ in (20).

We still must show that the $g_1(u,t)$ defined by (23) satisfies (13), if in (13) the $g_1(u,0)$ on the right is replaced by the given $g(u)$. To show this it suffices to show that if $Q(t)$ is computed from the $g_1(u,t)$ defined by (23), then the Laplace transform of

$$g(u)e^{-iku t} + ikv_p^2 g_0'(u) \int_0^t Q(\tau) e^{iku(\tau - t)}$$

is the $\gamma(u,s)$ of (20) with $g(u)$ replacing $g_1(u,0)$. But the Laplace transform of the integral in the foregoing expression is, by direct computation,

$$\frac{1}{ik(u-s)} \int_0^{\infty} Q(t) e^{iks t} dt,$$

which is $[ik(u-s)]^{-1} \int \gamma(u,s)du$ or, by (20), $-(kv_p)^{-2} \mathcal{L}(s)^{-1} (u-s)^{-1} \mathfrak{C}_u g_1(u,0)$. Comparison with (22) completes the proof that $g_1(u,t)$ satisfies (13).

V. CRITERION FOR THE STABILITY OF THE STEADY DISTRIBUTION

The initial distribution $g_0(u)$ is stable if all disturbances $g_1(u,t)$ of $g_0(u)$ remain bounded for all time. Whether $g_0(u)$ is stable thus depends on what we mean by "all" disturbances and what we mean by "bounded." When is a disturbance $g_1(u,0)$ to be regarded as physically realizable (disturbances whose initial electrostatic energy is infinite, for example, are of no physical interest), and what measure of the "size" of $g_1(u,t)$ is of interest in the particular problem at hand?

As for the first question, we have already agreed not to admit to consideration any disturbance $g_1(u,t)$ for which (11) or (12) fails, and we have discussed the reasons for this. We might make further demands on the smoothness of $g_1(u,0)$; for example, that $g_1(u,0)$ be square integrable, or bounded, or of bounded variation, or analytic in a strip $|\Im u| \leq a$ in the complex u plane. This last demand could be restated as the demand that for real u, $g_1(u,0)$ is infinitely differentiable and

$$\limsup_{n \to \infty} \left| \frac{g_1^{(n)}(u,0)}{n!} \right|^{1/n} \leq \frac{1}{a}.$$

In general, if we are trying to prove that $g_0(u)$ is stable, we will want to prove its stability against disturbances as rough as possible; if we are trying to prove that $g_0(u)$ is unstable, we will want to produce disturbances as smooth as possible which grow with time.

As for the second question, finding a measure of the "size" of $g_1(u,t)$, Landau has proposed the $Q(t)$ of Eq. (10), which is, except for a factor involving k, the amplitude of the electrostatic voltage produced by the given disturbance of the charge distribution. A second measure of the size of $g_1(u,t)$ is the $A(t)$ of Eq. (11), which is, except for the same factor involving k, the amplitude of the electrostatic voltage that would be produced if the electron distribution were $g_0(u) + |g_1(u,t)|$. Van Kampen[2] has considered a third measure, $\|g_1(u,t)\|_2$. Finally, $\|\partial g_1/\partial u\|_1$ might be considered, as when this number is large compared with $\|g_0'(u)\|_1$ the linear theory is no longer valid.

Landau's choice of $Q(t)$ to measure the size of $g_1(u,t)$ might be justified by noting that the electrostatic potential is what is observed. In principle, however, the

whole electron distribution is observable. Further, it is possible to have $g_1(u,t)$ very large in comparison with $g_0(u)$ and yet to have $Q(t)=0$. Therefore we reject $Q(t)$.

Three advantages lead us to adopt $A(t)$ as the measure of the size of $g_1(u,t)$. First, if $A(t)=0$, $g_1(u,t)=0$. Second, if $A(0)$ is finite, Eq. (13) has a unique solution for which $A(t)$ remains finite, so that $A(t)$ is a mathematically natural norm. Third, the finiteness of $A(t)$ has the clear physical significance that the charge density should be independent of the order in which the electrons are counted.

Van Kampen's suggestion, $\|g_1(u,t)\|_2$, has the first advantage enumerated in the foregoing and also the second if $g_0'(u)$ is bounded, but as Van Kampen himself points out, it is difficult to see the physical significance of this norm.

Finally, the norm $\|\partial g_1/\partial u\|_1$ will be discussed in Sec. VIII.

In summary, the steady distribution $g_0(u)$ will be called stable if for every initial disturbance $g_1(u,0)$, $\|g_1(u,t)\|_1=A(t)$ remains bounded for all time. It will be necessary to examine how unstable distributions become stable as more smoothness demands are made on the admissable initial disturbances. These ambiguities in the definition of stability come, of course, from the fact that the idealized physical system in question has an infinite number of degrees of freedom.

Besides the three lemmas enumerated in Sec. IV, we will need six more concerning $\mathcal{K}_{su}$.

Lemma 4: If $\Im s>0$ and $\|f(u)\|_1<\infty$, $|\mathcal{K}_{su}f(u)| \leq(\Im s)^{-1}\|f(u)\|_1$. If also in a neighborhood of the real point x, $f(u)$ is absolutely continuous and $f'(u)$ is bounded, then $\mathcal{K}_{su}f(u)$ is continuous as s approaches x from the upper complex s half-plane, and its limit is $\mathcal{P}\int_{-\infty}^{\infty}(u-x)^{-1}f(u)du+\pi i f(x)$, where $\mathcal{P}$ denotes the Cauchy principal part. If also $f(u)$ is absolutely continuous and $f'(u)$ is bounded for all u, then $\mathcal{K}_{x+iy,u}f(u)$ approaches the above limit uniformly in x as y approaches zero through positive values.

This lemma is proved, in a slightly different form, by Muskhelishvili.[3]

Lemma 5: If $\|f(u)\|_2<\infty$, and $y\geq 0$ then $\|\mathcal{K}_{su}f(u)\|_{y2} \leq 2\pi\|f(u)\|_2$. Furthermore, as $y\to 0$ through positive values, $\mathcal{K}_{x+iy,u}f(u)\to\mathcal{P}\int_{-\infty}^{\infty}(u-x)^{-1}f(u)du+\pi i f(x)$ for almost every x and also in the mean square.

Lemma 5 is proved by Titchmarsh.[4]

Lemma 6: Suppose $f(s)$ is a bounded analytic function of the complex variable s in the region $-b\leq\Im s\leq 0$, where b is a positive. Suppose that each of $f(x)$ and $f(x-ib)$ is either integrable or square integrable as a function of the real variable x. Then $\mathcal{K}_{su}f(u)$ can be extended analytically to the region $\Im s\geq -b$, and there

$$\mathcal{K}_{su}f(u)=\int_{-\infty-ib}^{\infty-ib}\frac{f(s')}{s'-s}ds'.$$

Lemma 6 is a consequence of Cauchy's theorem.

Lemma 7: If m and n are positive integers, and u, v, and b are real,

$$\int_{-\infty+ib}^{\infty+ib}\frac{ds}{|u-s|^m|v-s|^n} =\frac{2\pi}{(2b)^{m+n-1}}\binom{2m-2}{m-1}^{\frac{1}{2}}\binom{2n-2}{n-1}^{\frac{1}{2}},$$

where the usual notation for the binomial coefficients is used.

This lemma is simply Schwarz's inequality.

Lemma 8: Suppose $M(u)$ is square integrable. Then there exist unique functions $M_+(s)$ and $M_-(s)$ with these properties:

(i) $M_+(s)$ is analytic for $\Im s>0$, and $M_-(s)$ for $\Im s<0$;
(ii) there is a K such that $\|M_+(s)\|_{y2}\leq K$ for all $y>0$ and $\|M_-(s)\|_{y2}\leq K$ for all $y<0$;
(iii) $M(u)=M_+(u)+M_-(u)$ for almost every real u.

It should be noted that if $M_+(s)$ satisfies (ii) above, then $\lim_{y\to 0+}M_+(x+iy)$ exists for almost every real x and also in the mean square (Titchmarsh), and similarly for M_-, so that (iii) makes sense. It should also be noted that if condition (ii) is abandoned, $M_+(s)$ and $M_-(s)$ are no longer unique. For example, if $M(u)=\exp(-\frac{1}{2}u^2)$, $M_+(s)=\alpha\exp(-\frac{1}{2}s^2)$ and $M_-(s)=(1-\alpha)\exp(-\frac{1}{2}s^2)$ have properties (i) and (iii), but not (ii) for any real α.

Lemma 9: The $M_+(s)$ and $M_-(s)$ of lemma 8 have these properties:

(i) $$M_\pm(s)=\pm\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{M(u)}{u-s}du.$$

(ii) $$M_\pm(x)=\tfrac{1}{2}M(x)\pm\frac{1}{2\pi i}\mathcal{P}\int_{-\infty}^{\infty}\frac{M(u)}{u-x}du$$

for almost every real x. Here $\mathcal{P}$ means that the integral is to be interpreted as the Hilbert transform.

(iii) if $$m(k)=\text{l.i.m.}_{\lambda\to\infty}\frac{1}{\sqrt{2\pi}}\int_{-\lambda}^{\lambda}e^{-iku}M(u)du$$

then

$$m_+(x)=\text{l.i.m.}_{\lambda\to\infty}\frac{1}{\sqrt{2\pi}}\int_{0}^{\lambda}e^{ikx}m(k)dk$$

and

$$m_-(x)=\text{l.i.m.}_{\lambda\to\infty}\frac{1}{\sqrt{2\pi}}\int_{-\lambda}^{0}e^{ikx}m(k)dk.$$

(iv) $\|M_+(x)\|_2\leq\|M(x)\|_2$; $\|M_-(x)\|_2\leq\|M(x)\|_2$.

[3] N. I. Muskhelishvili, *Singular Integral Equations* (P. Noordhoff N.V., Groningen, 1953), Chap. 2, p. 38.
[4] E. C. Titchmarsh, *Introductions to the Theory of Fourier Integrals* (Oxford University Press, New York, 1948), 2nd ed., Chap. 5.

Our first stability theorem is a sufficient condition for instability.

Theorem 1: Let $s_1, \cdots, s_n, \cdots$ be the zeros of $\mathcal{L}(s)$ in the open upper s half-plane. Let a be any positive real number different from $s_1, \cdots, s_n, \cdots$ (the set of such a's is dense among positive numbers because the zeros of $\mathcal{L}(s)$ form a finite or denumerable set). Let $s_1, \cdots, s_N$ be the zeros for which $\Im s > a$ (N is finite by lemma 3). Let their multiplicities be $\nu_1, \cdots, \nu_N$. Then there is a positive number α such that $|\mathcal{L}(s)| \geq \alpha$ if $\Im s = a$, and for any integrable initial disturbance $g_1(u,0)$ there are functions $Q_{mn}(u)$ such that

$$g_1(u,t) = g_1(u,0)e^{-iku t} + \sum_{n=1}^{N} e^{-iks_n t} \sum_{m=1}^{\nu_n} Q_{mn}(u)t^{m-1} + g_a(u,t), \quad (24)$$

where

$$|g_a(u,t)| \leq \frac{g_0'(u)}{2\pi}\left(\frac{A(0)}{\alpha a}\right)e^{kat}.$$

Furthermore, $g_1(u,0)$ can be so chosen that it is integrable, square integrable, and analytic in a strip $|\Im u| \leq a'$ of positive width $2a'$, while $Q_{mn}(u) \neq 0$ if $m = \nu_n$.

It should be recalled that we always assume that $g_0'(u)$ is integrable. The existence of the α mentioned in the theorem is an immediate consequence of lemma 3. Then Eq. (24) and the bound on g_a are obtained by moving the contour of s integration in (23) down from the line $\Im s = b > v_p$ to the line $\Im s = a$. The sum in (24) comes from the poles of the integrand, and g_a is the integral along $\Im s = a$. The deformation of the contour of integration is justified by lemmas 1, 2, 3, 4, and 6, while lemmas 2 and 3 alone give the bound on g_a. If $g_0'(u)$ is analytic in a strip $|\Im u| \leq a'$, the functions $g_1(u,0)$ for which $Q_{mn}(u)$ is not zero can be obtained very simply by setting $t = 0$ in the following formula:

$$g_1(u,t) = \left(\frac{\partial}{\partial s}\right)^{m-1}\left(\frac{v_p^2 g_0'(u)e^{-iks t}}{u-s}\right). \quad (25)$$

When g_0' is integrable and s is a zero of $\mathcal{L}(s)$ in the open upper half-plane with order at least m, (25) is an exact solution of (8) and from it $Q(t) = (-ikt)^{m-1}e^{-iks t}/(m-1)!$. However, if $g_0'(u)$ is not analytic in a strip, the foregoing $g_1(u,0)$ is not, and we must make a different choice. We note that for any integrable $g_1(u,0)$, if $m = n$,

$$Q_{mn}(u) = \frac{-g_0'(u)m(-ikt)^{m-1}\mathcal{K}_{s_n v}g_1(v,0)}{(u-s_n)\mathcal{L}^{(m)}(s_n)},$$

so that all that is required is to find a function $g_1(u,0)$ analytic in a strip $|\Im u| \leq a'$ and such that $\mathcal{K}_{s_n v}g_1(v,0) \neq 0$. By lemmas 8 and 9, if $h(s)$ is a function analytic in $\Im s \geq -a'$ and such that $\|h(s)\|_{v^2} \leq K$ for some fixed K and all $y \geq -a'$, then $g_1(u,0) = \pi\Im h(u)$ has $\mathcal{K}_{su}g_1(u,0) = h(s)$. Therefore, all we need is a function $h(s)$ of the afore-mentioned sort with the further properties that $h(s_n) \neq 0$ and that $h(u)$ is integrable for real u. Obviously, many such functions are available, for example $(s+ia')^{-4}$, and $i(a'^2+s^2+\beta \exp s^2)^{-1}$, where the positive constant β is chosen so that the function does not vanish at s_n.

Theorem 1 really does nothing more than to make precise Landau's[1] assertion that $g_0(u)$ is unstable if $\mathcal{L}(s)$ has zeros in the upper half-plane. Landau tries to conclude the converse directly from (22); he argues that if $\mathcal{L}(s)$ has no zeros in the upper half-plane, the Laplace transform $\gamma(u,s)$ of every disturbance $g_1(u,t)$ is analytic in the upper s half-plane, or the right p half-plane, so that $g_1(u,t)$ must be bounded in time. This argument is at fault in assuming that if a function $f(t)$ has a Laplace transform which is analytic in the right p half-plane, $f(t)$ is bounded. Widder[5] shows that the Laplace transform of $e^t \sin e^t$ is an entire function of p.

One valid sufficient condition for stability is given by

Theorem 2: Suppose $g_0'(u)$ and $g_1(u,0)$ are integrable and square integrable. Suppose there is a positive number α such that $|\mathcal{L}(s)| \geq \alpha$ in the open upper s half-plane. Then $A(t) = \|g_1(u,t)\|_1$ is bounded for all time and, if $g_0'(u)$ is bounded, $\|g_1(u,t)\|_2$ is also bounded for all time.

Because of lemmas 1, 2, 3, 4, and 6 and the fact that $|\mathcal{L}(s)| \geq \alpha$, we can move the contour of integration in (23) down arbitrarily close to the x axis. Thus when $|\mathcal{L}(s)| \geq \alpha$, (23) is correct for any positive b. But by lemma 5

$$\|\mathcal{L}(s)^{-1}e^{-iks t}\mathcal{K}_{sv}g_1(v,0)\|_{b2} \leq 2\pi\alpha^{-1}e^{kbt}\|g_1(v,0)\|_2.$$

Therefore, the integral on the right in (23) is obtained from the foregoing function of s, square integrable on the line $\Im s = b$, by an operator like $\mathcal{K}_{su}$, except that the integration is along the line $\Im s = b$ instead of the real axis, and the argument of the function produced by the operator is real. Then lemma 5 can be applied, and as a function of u the integral on the right in (23) is square integrable, and the square root of the integral of its square is not larger than $(2\pi)^2\alpha^{-1}e^{kbt}\|g_1(v,0)\|_2$. When the whole term on the far right in (23) is integrated with respect to u, the result is the Hilbert space inner product of two square integrable functions of u, $g_0'(u)$ and the s integral. Hence, by Schwarz's inequality,

$$\|g_1(u,t)\|_1 \leq \|g_1(u,0)\|_1 + 2\pi\alpha^{-1}\|g_0'(u)\|_2\|g_1(u,0)\|_2 e^{kbt}. \quad (26)$$

Since (26) is true for all positive b, it is true for $b = 0$, which proves that $\|g_1(u,t)\|_1$ is bounded.

When $|g_0'(u)| \leq M$ for all u, the whole term on the far right in (23) is a square integrable function of u since the s integral is. Thus

$$\|g_1(u,t)\|_2 \leq \|g_1(u,0)\|_2 + 2\pi\alpha^{-1}M\|g_1(u,0)\|_2 e^{kbt}$$

for all positive b, and hence for $b = 0$.

[5] D. V. Widder, *The Laplace Transform* (Princeton University Press, Princeton, New Jersey, 1946), Chap. 2, p. 58.

One consequence of theorem 2 should be noted. If a disturbance $g_1(u,0)$ is integrable and bounded, it is square integrable, so that theorem 2 assures us that its $A(t)$ is bounded in time if $g_0(u)$ satisfies the hypotheses of theorem 2. We may still ask, what happens if either $g_0'(u)$ or $g_1(u,0)$ is not as smooth as is required in theorem 2. Theorem 3 and theorem 4 deal with this question.

Theorem 3: If $g_0(u)$ satisfies the conditions of theorem 2 there are integrable initial disturbances $g_1(u,0)$ for which $\|g_1(u,t)\|_1 = A(t)$ is not a bounded function of time.

To prove theorem 3, we write $s=x+iy$. Then

$$\mathcal{H}_{su}g_0'(u) = \int_{-\infty}^{\infty} \frac{(u-x)g_0'(u)du}{[(u-x)^2+y^2]^{\frac{1}{2}}} + iy\int_{-\infty}^{\infty} \frac{g_0'(u)du}{[(u-x)^2+y^2]^{\frac{1}{2}}}. \quad (27)$$

But by lemma 5, for almost every x, $\Im\mathcal{H}_{x+iy,u}g_0'(u) \to \pi g_0'(x)$ as $y \to 0$ through positive values. Hence we can find a real w such that

$$\lim_{y\to 0+} y\int_{-\infty}^{\infty} \frac{g_0'(u)du}{[(u-w)^2+y^2]^{\frac{1}{2}}} = \pi g_0'(w) \neq 0. \quad (28)$$

Then choose $g_1(u,0) = (u-w)^{-1}|\ln(u-w)|^{-\frac{3}{2}}$ if $w<u \leq w+\frac{1}{2}$ and $g_1(u,0)=0$ for all other u. Clearly, $g_1(u,0)$ is integrable, although not square integrable. Furthermore,

$$\mathcal{H}_{su}g_1(u,0) = \int_0^{\frac{1}{2}} \frac{du}{(u-s+w)u|\ln u|^{\frac{3}{2}}}.$$

If $s=w+iy$, then since the magnitude of a complex number is not less than its imaginary part,

$$|\mathcal{H}_{su}g_1(u,0)| > y\int_0^{\frac{1}{2}} \frac{du}{(u^2+y^2)u|\ln u|^{\frac{3}{2}}}.$$

When $y<\frac{1}{2}$,

$$|\mathcal{H}_{su}g_1(u,0)| > \frac{1}{2y}\int_0^{\frac{1}{2}} \frac{du}{u|\ln u|^{\frac{3}{2}}} = \frac{1}{y|\ln y|^{\frac{1}{2}}}.$$

Now let

$$K(s) = \int_{-\infty}^{\infty} \left| \frac{g_0'(u)}{u-s} \frac{\mathcal{H}_{sv}g_1(v,0)}{\mathfrak{L}(s)} \right| du. \quad (29)$$

Then if $s=w+iy$,

$$|K(s)| \geq \frac{1}{\alpha y|\ln y|^{\frac{1}{2}}} \int_{-\infty}^{\infty} \left|\frac{g_0'(u)}{u-s}\right| du \geq \frac{1}{\alpha y^2|\ln y|^{\frac{1}{2}}} y\int_{-\infty}^{\infty} \frac{g_0'(u)}{[(u-w)^2+y^2]^{\frac{1}{2}}}.$$

Thus, by (28), if y is sufficiently small and $s=w+iy$,

$$|K(s)| > \frac{\pi|g_0'(w)|}{2\alpha y^2|\ln y|^{\frac{1}{2}}}. \quad (30)$$

Suppose now that for the $g_1(u,0)$ defined in the foregoing, $A(t)$ is bounded, say $|A(t)| \leq m$ for all t. Then

$$\int_{-\infty}^{\infty} du \left| \int_0^{\infty} e^{ikst} g_1(u,t)dt \right| \leq \int_0^{\infty} dt \exp(-kt\Im s)\|g_1(u,t)\|_1 \leq m(k\Im s)^{-1},$$

or $k\int|\gamma(u,s)|du \leq m(\Im s)^{-1}$. From Eq. (22) and a standard inequality for Laplace transforms, it follows that $|K(s)| \leq 2m(\Im s)^{-1}$. This contradiction with (30) forces us to conclude that the $g_1(u,0)$, defined previously, generates a $g_1(u,t)$ for which $A(t)$ is not bounded.

Finally, we have

Theorem 4: Suppose that $g_0'(u)$ is integrable and that there is a positive number α such that $|\mathfrak{L}^{-1}(s)| \leq \alpha^{-1}$ if $\Im s>0$, while $|d\mathfrak{L}^{-1}(s)/ds| \leq \alpha^{-1}$ in a strip $0<\Im s<a$ for some positive a. Suppose that $g_1(u,0)$ is integrable and absolutely continuous and $g_1'(u,0)$ is integrable and bounded for all u. Then $A(t)$ is bounded.

Clearly, the contribution to $A(t)$ from the first term on the right in (23) is bounded, so we need consider only the integral. If we integrate this once by parts with respect to s and then integrate one of the resulting terms by parts with respect to v, we have for that integral the expression, valid for all positive b,

$$I = \frac{1}{ikt}\int_{-\infty+ib}^{\infty+ib} ds e^{-ikst}\left\{ \frac{\mathcal{H}_{sv}g_1'(v,0)}{(u-s)\mathfrak{L}(s)} + \frac{\mathcal{H}_{sv}g_1(v,0)}{(u-s)^2\mathfrak{L}(s)} + \frac{\mathcal{H}_{sv}g_1(v,0)}{(u-s)} \frac{d\mathfrak{L}^{-1}(s)}{ds} \right\}. \quad (31)$$

Now by lemma 2, the first term in braces contributes to the foregoing expression a quantity whose absolute value is

$$\leq \frac{\pi e^{kbt}}{kbt} \frac{\|g_1'(v,0)\|_1}{\alpha}.$$

Since $g_1(u,0)$ is bounded and, by lemma 4, $\mathcal{H}_{sv}g_1(v,0)$ has a bounded uniform limit as s approaches the real axis, it follows that there is a b so small that if $0 \leq \Im s < b$, $\mathcal{H}_{sv}g_1(v,0)$ is a bounded function of s, say $|\mathcal{H}_{sv}g_1(v,0)| \leq M$. Thus by lemma 7, the second term in (31) contributes to that expression a quantity whose absolute value is

$$\leq \frac{\pi e^{kbt}}{kbt} \frac{M}{\alpha}.$$

As for the third term, by lemma 5, and Schwarz's

inequality the absolute value of its contribution is

$$\leq \frac{\pi e^{kbt}}{kbt}\left(\frac{b}{\pi}\right)^{\frac{1}{2}} \frac{\|g_1(v,0)\|_2}{\alpha}$$

when $b<a$. It follows that when $b<a$,

$$I \leq \frac{e^{kbt}}{kbt}\frac{\pi}{\alpha}\|g_1'(v,0)\|_1 + M + \left(\frac{a}{\pi}\right)^{\frac{1}{2}}\|g_1(v,0)\|_2.$$

Since for fixed t, the foregoing inequality is true for all positive b, it is true in particular for $b=(kt)^{-1}$. Thus

$$I \leq \frac{e\pi}{\alpha}\|g_1'(v,0)\|_1 + M + \left(\frac{a}{\pi}\right)^{\frac{1}{2}}\|g_1(v,0)\|_2,$$

and then, from (23), $|A(t)| \leq A(0) + (2\pi)^{-1} I \|g_0'(u)\|_1$.

We see from theorem 3 that the square integrability of the initial disturbance is really necessary for stability, and we see from theorem 4 that the square integrability of $g_0'(u)$ is not necessary if we are willing to restrict our attention to absolutely continuous disturbances $g_1(u,0)$ with bounded derivatives.

Theorems 1, 2, 3, and 4 clearly leave a gap. What if $\mathfrak{L}(s)$ has zeros on the real axis, but none in the open upper half-plane? This question is partly answered by

Theorem 5: Suppose $g_0'(u)$ is integrable. Suppose there is a real w for which positive constants ν, ϵ, and M exist such that if $\Im s>0$ and $|s-w|<\epsilon$ then $|\mathfrak{L}(s)| \leq M|s-w|^{\nu+1}$. Then if a is any positive number and ν_1 is any positive number less than ν, there is an integrable, square-integrable initial disturbance $g_1(u,0)$, analytic in the strip $|\Im u| \leq a$, for which $t^{-\nu_1}|A(t)|$ is not bounded as $t \to \infty$.

The proof is rather like that of theorem 3. If $|A(t)| \leq mt^{\nu_1}$ then

$$\int_{-\infty}^{\infty} |\gamma(u,s)|\,du \leq \frac{m\Gamma(\nu_1+1)}{(k\Im s)^{\nu_1+1}}.$$

If $K(s)$ is defined by (29), then (22) and the foregoing inequality imply

$$|K(s)| < \frac{m\Gamma(\nu_1+1)}{(k\Im s)^{\nu_1+1}} + \frac{A(0)}{s}. \tag{32}$$

But if $s=w+iy$, then from its definition,

$$|K(s)| \geq \int_{-\infty}^{\infty} \frac{|g_0'(u)|\,du}{[(u-w)^2+y^2]^{\frac{1}{2}}} \frac{\mathfrak{K}_{sv}g_1(v,0)}{My^{\nu+1}}.$$

Thus

$$|K(s)| \geq \int_{-\infty}^{\infty} \frac{|g_0'(u)|\,du}{[(u-w)^2+1]^{\frac{1}{2}}} \frac{\mathfrak{K}_{sv}g_1(v,0)}{My^{\nu+1}}. \tag{33}$$

Now let $h(s)$ be any analytic function in $|\Im s| \leq a$ for which $\|h(s)\|_{\nu 2} \leq 1$ when $|y| \leq a$, and such that $h(w) \neq 0$. Then let $g_1(u,0)=\pi\Im h(u)$, so that $\mathfrak{K}_{sv}g_1(v,0)=h(s)$ by lemmas 8 and 9. If this $g_1(u,0)$ is used in (32), (32) and (33) are contradictory, so we conclude that $t^{-\nu_1}|A(t)|$ is not bounded.

Theorem 5 shows that if $\mathfrak{L}(s)$ has a zero of order greater than 1 on the real axis, $g_0(u)$ is unstable even to very smooth disturbances. However, if $\mathfrak{L}(s)$ has no zeros in the open upper half-plane and only a simple zero on the real axis, in general $g_0(u)$ will be stable to smooth disturbances and unstable to rough ones. The details are contained in theorems 6 and 7.

Theorem 6: Suppose $g_0'(u)$ is integrable and $g_0''(u)$ exists and is bounded in a neighborhood of each of the real points $w_1, \cdots, w_N$. Suppose that

$$\mathfrak{L}(s)^{-1} = \sum_{n=1}^{N} B_n(w_n-s)^{-1} + \mathfrak{M}(s)$$

and that there are positive constants a and α such that $|\mathfrak{M}(s)| \leq \alpha$ if $\Im s \geq 0$ and $|\mathfrak{M}'(s)| \leq \alpha$ if $0 \leq \Im s \leq a$. Suppose that $g_1(u,0)$ is integrable and absolutely continuous and that $g_1'(u,0)$ is integrable and bounded. Then $A(t)$ is bounded for all time.

By the argument of theorem 4, $\mathfrak{M}(s)$ contributes only a bounded term to $A(t)$ through the integral in (23). Therefore

$$A(t) = H_0(t) + \int du\ \Big|\sum_{n=1}^{N} B_n H_n(u,t)\Big|$$

where $H_0(t)$ is bounded and

$$H_n(u,t) = -\frac{g_0'(u)}{2\pi kt}\int_{-\infty+ib}^{\infty+ib} ds e^{-ikst} \frac{\mathfrak{K}_{sv}g_1'(v,0)}{(u-s)(w_n-s)} + \frac{\mathfrak{K}_{sv}g_1(v,0)}{(u-s)^2(w_n-s)} + \frac{\mathfrak{K}_{sv}g_1(v,0)}{(u-s)(w_n-s)^2}.$$

Here the same integrations by parts have been carried out as those described in the proof of theorem 4. Now by lemma 4 there are positive numbers m and a_1 such that if $0 \leq \Im s < a_1$, $|\mathfrak{K}_{su}g_1(u,0)| < m$. Further $(u-s)^{-1}(w_n-s)^{-1} = (u-w_n)^{-1}[(w_n-s)^{-1}-(u-s)^{-1}]$, and $(u-s)^{-2}(w_n-s)^{-1} = (u-w_n)^{-1}[(u-s)^{-1}(w_n-s)^{-1}-(u-s)^{-2}]$ and $(u-s)^{-1} \times (w_n-s)^{-2} = -(u-w_n)^{-1}[(u-s)^{-1}(w_n-s)^{-1} - (w_n-s)^{-2}]$. Finally, by lemma 4, $g_0'(u)$ has a zero of at least first order at $u=w_n$, so $M = \int |g_0'(u)|\,|u-w_n|^{-1}du < \infty$. Therefore

$$\int_{-\infty}^{\infty} |H_n(u,t)|\,du \leq \frac{e^{kbt}}{kbt} M[2\pi\|g_1'(v,0)\|_2 + 2m].$$

Since this inequality is true for all positive b less than a', it is true for $b=(kt)^{-1}$ when t is large. Thus $A(t)$ is bounded.

If $g_1(u,0)$ is not as smooth as in theorem 6, the result of that theorem is no longer true, as we see from

Theorem 7: Suppose $g_0'(u)$ is integrable. Suppose there exist positive numbers α and ϵ and a real w such that $g_0'(u)$ is analytic for complex u in $|u-w|<\epsilon$, while

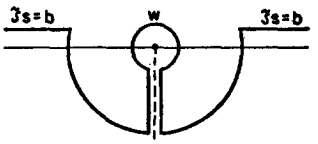

FIG. 1. Deformed contour of integration for Eq. (34). The dotted line is a cut in the complex s plane.

$|\mathcal{L}(s)|\geq\alpha$ if $|s-w|\geq\epsilon$ and $\Im s>0$. Suppose further that $\mathcal{L}(s)^{-1}=(s-w)^{-1}\mathfrak{N}(s)$ and that $\mathfrak{N}(w)\neq 0$. Then for any m in $0<m<\frac{1}{2}$, there is an integrable, square integrable $g_1(u,0)$ for which the charge density $Q(t)$ behaves like t^m when t is large.

We take $g_1(u,0)=\pi^{-1}\Im[(u-w)^{-m}(u+i)^{-2}]$, where the fractional power is defined so as to be real and positive for large u and analytic in the complex upper u half-plane. Then by lemmas 8 and 9, $\mathfrak{IC}_{su}g_1(u,0)=(s-w)^{-m}(s+i)^{-2}$ if $\Im s>0$. We compute $Q(t)$ from (20) and the complex inversion formula for the Laplace transform:

$$Q(t)=\frac{1}{2\pi i v_p{}^2}\int_{-\infty+ib}^{\infty+ib}\frac{ds e^{-iks}t\mathfrak{N}(s)}{(s-w)^{m+1}(s+i)^2},\qquad(34)$$

where b is any positive number. By an extension of lemma 6, $\mathcal{L}(s)$ is analytic in the circle $|s-w|<\epsilon$, so the contour of integration in (34) can be deformed to that shown in Fig. 1, where the dotted line is a cut in the s plane. An integration by parts like that used in the proof of theorem 6 shows that the contribution to (34) from the horizontal lines and the large circular segments remains bounded as $t\to\infty$. The contribution from the small circle and the two vertical lines on opposite sides of the cut is computed by standard methods; then the radius of the small circle is allowed to approach zero for fixed t, and afterwards, t is allowed to become large. The resulting contribution to (34) is $-E(kt)^m+h(t)$, where $h(t)\to 0$ as $t\to\infty$, and

$$E=\left(\frac{\mathfrak{N}(w)(1-m)\sin\pi m}{(w+i)^2 v_p{}^2\pi m}\right)\exp\left[-i\left(\frac{\pi}{2}m+kwt\right)\right].$$

As this section makes clear, the stability of the steady distribution $g_0(u)$ depends heavily on how smooth are the disturbances which we admit as physically realizable. Theorems 5, 6, and 7 deal with the rather special case in which $\mathcal{L}(s)$ has zeros for which $\Im s=0$ but none for which $\Im s>0$. The result of the more important theorems 1 through 4 might be paraphrased very roughly as that if $\mathcal{L}(s)$ has zeros with $\Im s>0$, $g_0(u)$ is certainly unstable. If $|\mathcal{L}(s)|\geq\alpha>0$ in the upper half-plane, then $g_0(u)$ is stable if $g_0'(u)$ and $g_1(u,0)$ are smooth enough; and if one is roughened, stability can be preserved by smoothing the other.

VI. STABILITY OF SOME PARTICULAR STEADY DISTRIBUTIONS

Our theory is unable to treat the case $g_0(u)=\delta(u)$, where δ is the Dirac delta function. Theorems 1, 4, 5, 6, and 7 do, however, remain true if the demand that $g_0'(u)$ be integrable is replaced by the demand that $g_0(u)$ be of bounded variation, all other demands on $g_0(u)$ remaining as stated in those theorems. Although we have not proved this fact, the proof amounts to cumbersome but inessential modifications in the proofs already given. Therefore, the theory, with this slight extension, is applicable to the distribution defined as $g_0(u)=(2w)^{-1}$ if $|u|<w$, $g_0(u)=0$ if $|u|\geq w$. For this distribution, $\mathcal{L}(s)=v_p{}^{-2}-(w^2-s^2)^{-1}$. If k is chosen so small that $v_p{}^2>w^2$, $\mathcal{L}(s)$ has a pure imaginary zero at $i(v_p{}^2-w^2)^{\frac{1}{2}}$, and so $g_0(u)$ is unstable to disturbances of this wave number with analytic u dependence, the rate of growth of the instability being $(\omega_p{}^2-k^2w^2)^{\frac{1}{2}}$; as predicted in Sec. III, this is less than ω_p. If k is so chosen that $v_p=w$, $\mathcal{L}(s)$ has a double zero at $s=0$, so, by theorem 5, $g_0(u)$ is unstable to disturbances of this wave number as well. Finally, if $k>\omega_p w^{-1}$, $\mathcal{L}(s)$ has simple real zeros at $s=\pm(w^2-v_p{}^2)^{\frac{1}{2}}$. By theorems 6 and 7, $g_0(u)$ is stable to disturbances at these wave numbers if the disturbances are absolutely continuous functions of u with bounded derivatives, and becomes unstable if all integrable, square integrable disturbances are allowed.

As a second example, suppose that $g_0'(u)$ is integrable, square integrable, and absolutely continuous, and that $g_0''(u)$ is bounded. Suppose further that there is a w such that $g_0'(u)<0$ if $u>w$ and $g_0'(u)>0$ if $u<w$, so that $g_0(u)$ has a single maximum at $u=w$; we may, without loss of generality, take $w=0$. Then we can show that there is a positive α such that $|\mathcal{L}(s)|\geq\alpha$ in the open upper half-plane; therefore $g_0(u)$ is stable to integrable, square integrable disturbances and unstable to certain integrable disturbances (theorems 2 and 3). As the first step in the proof of these assertions, we note that, by lemma 4, when s is real $\mathcal{L}(s)=v_p{}^{-2}-\int(u-s)^{-1}g_0'(u)du-\pi i g_0'(s)$. Therefore the only possible real zero of $\mathcal{L}(s)$ is $s=0$, and $\mathfrak{R}\mathcal{L}(0)>0$. Therefore $\mathcal{L}$ has no real zeros. It is easy to see that as $s\to\pm\infty$ along the real axis, $\mathcal{L}(s)\to v_p{}^{-2}$, so there is a positive number $2\alpha_1$ such that $|\mathcal{L}(s)|>2\alpha_1$ if s is real. Referring again to lemma 4, $\mathcal{L}(x+iy)\to\mathcal{L}(x)$ uniformly in x as $y\to 0$ from above, so there is a positive number a such that if $0\leq\Im s\leq a$, $|\mathcal{L}(s)|\geq\alpha_1$. Let $\mathcal{Q}$ be the set of all s for which $\Im s\geq a$, and which lie in neither $C_1(\alpha_1)$ nor $C_2(\alpha_1)$ as those sets are defined in lemma 3. Then $\mathcal{Q}$ is a closed, bounded (compact) set and outside $\mathcal{Q}$, $|\mathcal{L}(s)|\geq\alpha_1$. But $|\mathcal{L}(s)|$ is continuous in $\mathcal{Q}$, so if it has no zero in $\mathcal{Q}$ there is a positive α_2 such that $|\mathcal{L}(s)|\geq\alpha_2$ if s is in $\mathcal{Q}$. In this situation we take $\alpha=\min(\alpha_1,\alpha_2)$ and conclude that $|\mathcal{L}(s)|\geq\alpha$ whenever $\Im s\geq 0$. Therefore it remains to show that $\mathcal{L}(s)\neq 0$ if s is in $\mathcal{Q}$. But whenever $\Im s>0$, it is clear from Eq. (27) that if $\Im\mathcal{L}(s)=0$ then

$$\mathfrak{R}\mathcal{L}(s)=v_p{}^{-2}-\int[(u-x)^2+y^2]^{-1}ug_0'(u)du>v_p{}^{-2}.$$

Therefore $\mathcal{L}(s)$ has no zeros with $\Im s\geq 0$, and certainly none in $\mathcal{Q}$.

Of course one of the most interesting cases of example 2 is example 3, the Maxwell distribution, $g_0(u) = (2\pi)^{-\frac{1}{2}}\sigma^{-1}\exp(-\frac{1}{2}u^2\sigma^{-2})$, where $\sigma = \kappa T/m$. The remarks of the preceding paragraph all apply to this distribution, so it is stable to integrable, square integrable disturbances and unstable to certain integrable disturbances which are not square integrable. It should be recalled that these results apply to disturbances of a single spatial wavelength. However, if $\iint |f_1(x,u,t)|\,dxdu$ were bounded, so would be our $\iint |f_1(k,u,t)|\,du = A(t)$ for each k. Hence physical disturbances f_1 for which $\iint |f_1(x,u,0)|\,dxdu < \infty$ can be unstable on the Maxwell distribution in the sense that $\iint |f_1(x,u,t)|\,dxdu$ is not bounded as t goes to infinity.

As a fourth example, consider a three-dimensional steady distribution $f_0(\mathbf{q})$ which is isotropic: $f_0(\mathbf{q}) = h(q^2)$. For such a distribution, $g_0(u) = \iint h(u^2+v^2+w^2)dvdw = 2\pi\int_0^\infty h(u^2+\rho^2)\rho d\rho$, or $g_0(u) = \pi\int_{u^2}^\infty h(x)dx$. Thus $g_0'(u) = -2\pi u h(u^2)$ and since $h>0$, $ug_0'(u)<0$. Then, as in example 2, $\mathfrak{L}(s)$ has no zeros with $\Im s \geq 0$. If $h(x)$ is absolutely continuous and $h(x)+2xh'(x)$ is bounded and $x^{\frac{1}{4}}h(x)$ is square integrable, then $g_0(u)$ is a special case of example 2, and is stable to all integrable, square integrable disturbances.

VII. VAN KAMPEN'S NORMAL MODES

So far the whole discussion of (8) has been based on the Laplace transform. Now we examine briefly another technique for the solution of (8) when $g_1(u,0)$ is given, namely the expansion of $g_1(u,0)$ in terms of the normal modes of the system. For a stable system, these normal modes would be expected to have the time dependence $e^{-i\omega t}$ where ω was real. For an unstable system, we might expect to have to include modes in which $\Im\omega > 0$. Nevertheless, Van Kampen[2] gives a solution of the initial value problem entirely in terms of modes with real ω, and never explicitly assumes that the steady distribution $g_0(u)$ with which he deals is stable. He has, however, implicitly made this restriction, as he considers only $g_0(u)$ which come from isotropic $f_0(\mathbf{q})$; we have seen in the preceding section that these are always stable, subject to a few smoothness conditions. In the present section we propose to generalize van Kampen's treatment to unstable distributions $g_0(u)$. We shall assume throughout the present section that $g_0'(u)$ and $g_1(u,0)$ are square integrable.

Following Van Kampen, we look for solutions of (8) whose time dependence is $e^{-iks t}$ for some s. Van Kampen shows that, if we admit solutions $g_1(u,t)$ so singular in their dependence on u that they must be treated as distributions in the sense of Schwartz,[6] then for every real s we can find exactly one (to within a constant factor) solution of (8), $g_1(u,t) = H(u,s)e^{-iks t}$, where

$$H(u,s) = g_0'(u)\mathcal{P}(u-s)^{-1} + \left[v_p^{-2} - \mathcal{P}\int_{-\infty}^{\infty}(v-s)^{-1}g_0'(v)dv\right]\delta(u-s). \quad (35)$$

Here the first $\mathcal{P}$ means that $(u-s)^{-1}$ is that distribution which, when applied to the infinitely differentiable test function $f(u)$, gives the Cauchy principal value of $\int_{-\infty}^{\infty}(u-s)^{-1}f(u)du$. Of course these singular solutions are not physically realizable; they are a mathematical device useful in solving (8). Van Kampen writes the general solution $g_1(u,t)$ of (8) as a superposition of the normal modes (35):

$$g_1(u,t) = \int_{-\infty}^{\infty} V(s)H(u,s)e^{-iks t}ds. \quad (36)$$

The weight $V(s)$ of the normal mode with frequency ks is determined from the singular integral equation obtained by putting $t=0$ in (36). To solve this singular integral equation, Van Kampen writes it in the form

$$G(u) = V_+(u)[v_p^{-2} + 2\pi i E_+(u)] + V_-(u)[v_p^{-2} - 2\pi i E_-(u)], \quad (37)$$

where $G(u) = g_1(u,0)$, $E(u) = -g_0'(u)$, and $V_+(s)$, $V_-(s)$, $E_+(s)$, $E_-(s)$ are obtained from the square integrable functions V and E by lemmas 8 and 9, Sec. V, of the present paper. (Van Kampen has, incidentally, omitted the essential condition (ii) from lemma 8.) Van Kampen argues that (37) is a representation of the square integrable function $G(u)$ in the form $G_+(u)+G_-(u)$ described by lemma 8, so that the uniqueness assertion in that lemma produces from (37) the two equations,

$$G_+(s) = V_+(s)[v_p^{-2} + 2\pi i E_+(s)] \quad \text{for} \quad \Im s > 0,$$

and

$$G_-(s) = V_-(s)[v_p^{-2} - 2\pi i E_-(s)] \quad \text{for} \quad \Im s < 0.$$

Since $G_\pm(s)$ and $E_\pm(s)$ are known, these equations can be solved for $V_\pm(s)$; and when s is real, $V(s) = V_+(s) + V_-(s)$.

As Van Kampen points out, if $v_p^{-2} + 2\pi i E_+(s)$ has a zero in the upper half-plane, $G_+(s)[v_p^{-2} + 2\pi i E_+(s)]^{-1}$ is not analytic there, and so cannot be $V_+(s)$. Therefore, if $v_p^{-2} + 2\pi i E_+(s)$ has zeros in the upper half-plane, the general solution of (8) cannot be represented in the form (36). Similar remarks apply to $v_p^{-2} - 2\pi i E_-(s)$ and the lower half-plane. By using the assumption that $f_0(\mathbf{q})$ is isotropic, Van Kampen proves that $v_p^{-2} \pm 2\pi i E_\pm(s) \neq 0$ in the upper (lower) half-plane, justifying (36).

In the rest of Sec. VII and only in this section, let us denote by $\mathfrak{L}^+(s)$ the function defined by (21) when $\Im s > 0$, and by $\mathfrak{L}^-(s)$ the function defined by (21) when $\Im s < 0$. Then $\mathfrak{L}^-(s^*) = \mathfrak{L}^+(s)^*$ since $g_0'(u)$ is real, but when s is real $\mathfrak{L}^-(s) \neq \mathfrak{L}^+(s)$, as is clear from lemma 9. In the preceding sections, $\mathfrak{L}^+(s)$ has been called simply

[6] L. Schwartz, *Théorie des Distributions* (Hermann & Cie, Paris, France, 1950), Vol. I.

$\mathfrak{L}(s)$. As a consequence of lemma 9

$$\mathfrak{L}^+(s)=v_p^{-2}+2\pi i E_+(s) \quad \text{if} \quad \Im s>0 \tag{38}$$

and

$$\mathfrak{L}^-(s)=v_p^{-2}-2\pi i E_-(s) \quad \text{if} \quad \Im s<0. \tag{39}$$

Clearly, Van Kampen's proof that the right side of (38) has no zero in the upper half-plane is really another proof that isotropic steady distributions are stable.

We must now investigate how (36) is to be modified when $g_0(u)$ is unstable. For simplicity, we restrict ourselves to the case in which there is a positive α such that $|\mathfrak{L}^+(s)|\geq\alpha$ if $\Im s\geq 0$, except in neighborhoods of finitely many points $s_1, \cdots, s_N$, which are zeros of $\mathfrak{L}(s)$ with respective orders $\nu_1, \cdots, \nu_N$.

As we have already seen in equation (25), if $n=1, \cdots, N$ and $m=1, \cdots, \nu_N$, then

$$g_{nm}(u,t)=\frac{v_p^2 g_0'(u)e^{-iks_nt}}{(u-s_n)^m}\sum_{q=0}^{m-1}\frac{[ikt(s_n-u)]^q}{q!}$$

is an exact solution of (8). If we replace s_n by s_n^* in the above formula, we get another exact solution of (8), $h_{nm}(t)$, because s_n^* is a zero of $\mathfrak{L}^-(s)$ of order ν_n; $h_{nm}(t)$ is damped in time if s_n is not real. We suspect that the modes g_{nm} and h_{nm} ought to be included in the general solution $g_1(u,t)$ of (8), so we try to write that solution in the form

$$g_1(u,t)=\int_{-\infty}^{\infty}V(s)H(u,s)e^{-iks t}ds + \sum_{n=1}^{N}\sum_{m=1}^{\nu_n}[C_{nm}g_{nm}(u,t)+D_{nm}h_{nm}(u,t)], \tag{40}$$

where $V(s)$ and the coeff C_{nm} and D_{nm} are to be determined from the given function $g_1(u,0)=G(u)$. Clearly, if we can find $V(s)$, C_{nm}, and D_{nm} at all, they will depend linearly on $G(u)$, so it suffices to consider only real $G(u)$. If we set $t=0$ in (40), we obtain, in the notation of (37), (38), and (39),

$$H(u)=V_+(u)\mathfrak{L}^+(u)+V_-(u)\mathfrak{L}^-(u), \tag{41}$$

where

$$H(u)=G(u)-v_p^2 \times\sum_{n=1}^{N}\sum_{m=1}^{\nu_n}\left[C_{nm}\frac{g_0'(u)}{(u-s_n)^m}+D_{nm}\frac{g_0'(u)}{(u-s_n^*)^m}\right]. \tag{42}$$

If we can choose the const C_{nm} and D_{nm} so that $H_+(s)$ has a zero of order $\geq\nu_n$ at s_n and $H_-(s)$ has a zero of $\geq\nu_n$ at s_n^*, $n=1, \cdots, N$, then the functions $\mathfrak{L}^+(s)^{-1}H_+(s)$ and $\mathfrak{L}^-(s)^{-1}H_-(s)$ will satisfy conditions (i) and (ii) of lemma 8, and therefore will be the $V_+(s)$ and $V_-(s)$ of some square integrable function $V(x)$ of the real variable x which can then be found as $V(x)=V_+(x)+V_-(x)$.

Thus we want to choose C_{mn} and D_{mn} in such a way that the expression

$$\int_{-\infty}^{\infty}\frac{G(u)}{u-s}du-v_p^2\sum_{n=1}^{N}\sum_{m=1}^{\nu_n}\left[C_{nm}\int_{-\infty}^{\infty}\frac{g_0'(u)du}{(u-s)(u-s_n)^m}+D_{nm}\int_{-\infty}^{\infty}\frac{g_0'(u)du}{(u-s)(u-s_n^*)^m}\right]$$

has zeros of order ν_n at s_n and s_n^*, $n=1, \cdots, N$. From the equation

$$\frac{1}{(u-s)(u-s_n)^m}=\frac{1}{(s-s_n)^m(u-s)}-\sum_{q=1}^{m}\frac{1}{(s-s_n)^{m+1-q}(u-s_n)^q}$$

and the fact that $\mathfrak{L}^+(s)$ and its first ν_n-1 derivatives vanish at s_n, it follows that

$$\int_{-\infty}^{\infty}\frac{g_0'(u)du}{(u-s)(u-s_n)^m}=-\frac{\mathfrak{L}^{\pm}(s)}{(s-s_n)^m}, \tag{43}$$

where $\mathfrak{L}^+$ is used if $\Im s>0$ and $\mathfrak{L}^-$ is used if $\Im s<0$. Equation (43) remains true if s_n is replaced by s_n^*. Therefore we must choose C_{nm} and D_{nm} so that

$$\frac{1}{\mathfrak{L}^+(s)}\int_{-\infty}^{\infty}\frac{G(u)}{u-s}du+v_p^2\sum_{n=1}^{N}\sum_{m=1}^{\nu_n}\left[\frac{C_{nm}}{(s-s_n)^m}+\frac{D_{nm}}{(s-s_n^*)^m}\right] \tag{44}$$

is analytic when $\Im s>0$, and that (44) with $\mathfrak{L}^+$ replaced by $\mathfrak{L}^-$ is analytic when $\Im s<0$. Therefore the coefficients C_{nm} and D_{nm} are given by

$$D_{nm}^*=C_{nm}=-\frac{1}{2\pi i v_p^2}\oint\frac{\mathcal{K}_{su}G(u)}{\mathfrak{L}^+(s)}(s-s_n)^{m-1}ds, \tag{45}$$

where the contour of integration encircles s_n in the positive direction and includes no other zeros of $\mathfrak{L}^+$. That (45) gives C_{nm} correctly is Cauchy's theorem, and D_{nm} is computed from (44) as a contour integral around s_n^*, which, because $G(u)$ is real, is the complex conjugate of the expression on the right in (45).

We have proved that the general solution of (8) is (40) when $g_1(u,0)=G(u)$ is square integrable and $\mathfrak{L}^+(s)$ has no real zeros. If $\mathfrak{L}^+(s)$ has real zeros our proof breaks down unless $G(u)$ is analytic in a neighborhood of each of those zeros so that the integral (45) can be evaluated.

The question might arise, $\mathfrak{L}^+(s)$ is defined by (21); may it not follow that all zeros of $\mathfrak{L}^+(s)$ are simple, so that the foregoing discussion can be much simplified. The answer is negative and follows immediately from lemmas 8 and 9. Any function $f(s)$ with properties (i) and (ii) of lemma 8 is $\mathcal{K}_{su}g_0'(u)$ for $g_0'(u)=\pi^{-1}\Im f(u)$, so by choosing an $f(s)$ which takes the value v_p^{-2} to order

ν_n at s_n, we produce an $\mathfrak{L}^+(s)$ with a zero of order ν_n at s_n.

One curious consequence of the fact that the $V(s)$ and C_{nm}, D_{nm} in (37) are determined uniquely by $g_1(u,0)$ (and we have proved this) is that the "normal modes" of this particular mechanical system, that is the solutions of (8) whose time dependence is $e^{-iks\,t}$ for some s, real or complex, do not form a complete set if $\mathfrak{L}^+(s)$ has repeated zeros. [*Note added in proof.* E. A. Frieman has called to the author's attention K. M. Case's paper, Annals of Physics **7**, 293 (1959), in which Case asserts the contrary. Case has apparently generalized from $^+(s)$ with simple zeros to those with multiple zeros, having examined only the former problem in detail.] And if $\mathfrak{L}^+(s)$ has repeated real zeros and no zeros with $\Im s>0$, Eq. (40) shows that all "normal modes" of the system are bounded, while there are also solutions $g_1(u,t)$ which grow like polynomials in time. In this special situation, a test for stability which consisted in looking for "normal modes" with $\Im s>0$ would lead to the erroneous conclusion that the system was stable.

VIII. VALIDITY OF THE LINEARIZATION

If the stability of a mechanical system is to be established by linearizing the equations of motion of that system, the argument must include a verification that if the neglected terms are initially small, they remain so forever. Even this is not a proof of stability, but it is the best one can do with the linearized equations, and a contrary result puts positive assertions about stability in very serious doubt. It is the contrary result which confronts us in the present instance.

Specifically, Eq. (4) was derived from Eq. (2) by neglecting $\mathbf{E}\cdot\partial f_1/\partial\mathbf{q}$ in comparison with $\mathbf{E}\cdot\partial f_0/\partial\mathbf{q}$. We will restrict our attention to one-dimensional disturbances, and will show that for steady distributions $g_0(u)$, which are stable in the sense of Sec. V [i.e., for which the *linear* Eq. (8) has no explosive solutions] $\partial g_1/\partial u$ grows linearly with time at a rate proportional to its initial amplitude.

To simplify the discussion, we assume that $g_1(u,0)$ and $g_0'(u)$ are analytic in a strip $|\Im u|\leq a$ in the complex u plane and that $\|g_0'(s)\|_{yn}$, $\|g_1(s,0)\|_{yn}$, and $\|g_1'(s,0)\|_{yn}$ are bounded for $|y|\leq a$ and $n=1,2$. We also assume that there is a positive α such that $|\mathfrak{L}^{-1}(s)|\leq\alpha$ and $|d\mathfrak{L}^{-1}/ds|\leq\alpha$ when $\Im s\geq -a$. These restrictions do not exclude that $g_0(u)$ be the Maxwell distribution.

If we differentiate (23) with respect to u, a term $(u-s)^{-2}$ will appear inside the integral; it can be reduced to $(u-s)^{-1}$ by an integration by parts with respect to s. If the contour of integration is then moved down to $\Im s=-a$, account being taken of the pole at $s=u$, the result is

$$\partial g_1(u,t)/\partial u=-ikt g_1(u,t)+h_1(u,t), \tag{46}$$

where $h_1(u,t)$, $\|h_1(u,t)\|_1$ and $\|h_1(u,t)\|_2$ are bounded. To show that $g_1(u,t)$ does not approach zero as $t\to\infty$, we return to (23) and move the contour of integration down to $\Im s=-a$, obtaining

$$g_1(u,t)=e^{-iku\,t}[g_1(u,0)+\mathfrak{L}^{-1}(u)g_0'(u)\mathfrak{C}_{uv}g_1(v,0)]+g_a(u,t), \tag{47}$$

where $g_a(u,t)$ behaves like e^{-akt} as $t\to\infty$. The fact that the smoothness requirements of the present section lead to an indefinitely prolonged oscillation in $g_1(u,t)$ was pointed out by Landau.[1]

From Eqs. (46) and (47) it is clear that $|\partial g_1/\partial u|$ grows linearly with time, and will eventually dominate $g_0'(u)$.

There appear to be two possible difficulties with the foregoing argument, neither of which is in fact a real difficulty. The first is that although $\partial g_1(u,t)/\partial u$ grows linearly with time, the term which has been neglected in the linearization of (2) is really $Q(t)\partial g_1(u,t)/\partial u$, $Q(t)$ being the electric field times a factor depending on k. When $g_1(u,0)$ is analytic in a strip $|\Im u|\leq a_1$ in the complex u plane, and $g_0(u)$ is a Maxwell distribution with rms thermal velocity σ, Landau[1] has shown that $Q(t)$ goes to zero exponentially with a decay rate which is the smaller of a_1k and

$$\epsilon=\omega_p(\pi/8)^{\frac{1}{2}}(k\lambda_D)^{-3}\exp[-\tfrac{1}{2}(k\lambda_D)^{-2}], \tag{48}$$

where $\lambda_D=\sigma/\omega_p$ is the Debye shielding length. We will assume that a_1 is so large that the decay rate is ϵ. Thus eventually $Q(t)\partial g_1(u,t)/\partial u$ becomes negligible as $t\to\infty$. In thermonuclear plasmas, however, ϵ is in fact so very small that this Landau damping will not have time to become effective before the linearization fails. To get an idea of the orders of magnitude involved, let $g_0(u)=(2\pi)^{\frac{1}{2}}\sigma^{-1}\exp(-\frac{1}{2}u^2/\sigma^2)$ and $g_1(u,0)=\beta(2\pi)^{-\frac{1}{2}}\sigma_1^{-1}\exp(-\frac{1}{2}(u-w)^2/\sigma_1^2)$ where w, σ, σ_1, β are positive constants. The expected size of β can be estimated by noting that β is the total charge density of the initial disturbance, so the electrostatic voltage produced by the initial disturbance is $\phi=4\pi Ne\beta k^{-2}$. In the velocity range $|u-w|\leq\sigma_1$, which contains most of the disturbed particles,

$$\left|\frac{g_1(u,0)}{g_0'(u)}\right|\approx\frac{\beta\sigma^3}{\sigma_1 w}\exp(w^2/2\sigma^2) \tag{49}$$

and

$$\left|\frac{\partial g_1(u,0)/\partial u}{g_0'(u)}\right|\approx\frac{\beta\sigma^3}{\sigma_1^2 w}\exp(w^2/2\sigma^2). \tag{50}$$

Since $|\partial g_1(u,t)/\partial u|\approx kt|g_1(u,0)|$, from (49)

$$\left|\frac{\partial g_1(u,t)/\partial u}{g_0'(u)}\right|\approx t\left(\frac{k\beta\sigma^3}{\sigma_1 w}\right)\exp(w^2/2\sigma^2) \tag{51}$$

when t is large. Unless $Q(t)$ has become very small, the linear theory fails when the term on the right becomes comparable to 1, i.e., when

$$\omega_p t\approx\frac{\sigma_1 w}{\sigma^2}\left(\frac{\kappa T}{e\phi}\right)\frac{\exp(-w^2/2\sigma^2)}{(k\lambda_D)^3}, \tag{52}$$

where κ is Boltzmann's constant and T is the temperature of g_0. If $T=10^4$ ev and $N=10^{15}$ cm^{-3}, as one might expect in a typical thermonuclear plasma, then $\lambda_D=2.4\times10^{-3}$ cm. For a disturbance in which ϕ is initially 1 v, $w=2\sigma$, $\sigma_1=\sigma/2$, and $k=2\pi$ cm^{-1}, (52) gives $\omega_p t\approx 4\times10^8$. Thus the linear theory will be valid for about 6×10^7 plasma oscillations or about 2.2×10^{-4} sec, since $\omega_p=1.8\times10^{12}$ sec^{-1}. The Landau damping rate (48) is, in the present instance, about $\exp(-2.3\times10^3)$ sec^{-1}, so that no observable Landau damping occurs. It should be noticed, incidentally, that our choice $\phi=1$ v makes β so small that the right side of (50) is much less than 1, which is the condition for the applicability of the linear theory near time $t=0$.

The second possible difficulty with the foregoing argument that the linear theory eventually fails is that the discussion so far has been restricted to disturbances whose initial x dependence involved a single pure wave number. Will the argument still be valid for real disturbances with broad wave-number spectra? That it will can be seen immediately from (46) and (47). If we take inverse Fourier transforms with respect to k in (46), we obtain

$$f_1(x,u,t)=\hat{f}(x-ut,\,u)+f_a(x,u,t), \tag{53}$$

where

$$\hat{f}(x,u)=\tfrac{1}{2}\pi\int_{-\infty}^{\infty}[g_1(k,u,0)+\mathfrak{L}^{-1}(k,u)g_0'(u)\mathfrak{K}_{uv}g_1(k,v,0)]e^{ikx}dk \tag{54}$$

and $\partial f_a/\partial u$ is bounded as $t\to\infty$. The convergence of the integral defining $\hat{f}(x,u)$ is assured by the assumptions made at the beginning of the present section, and in fact $\hat{f}(x,u)$ is integrable with respect to u and square integrable with respect to x. Obviously $\partial f_1/\partial u$ is linear in t for large t.

IX. CONCLUSIONS

In a collisionless plasma whose protons are fixed and whose electrons have a steady Boltzmann distribution function $g_0(u)$ with integrable derivative, we have shown (Sec. III) that no disturbance $g_1(k,u,t)$ in the electrons' distribution can grow too rapidly to have a Laplace transform, and in fact that none has a growth rate larger than the plasma frequency of the steady distribution. We have then shown (Sec. IV) that if $g(u)$ is integrable, the linearized Boltzmann equation has a solution $g_1(u,t)$ for which $g_1(u,0)=g(u)$, and we have shown that Landau's expression for that solution is valid; it is not necessary to assume that $g_0(u)$ and $g(u)$ are analytic in a strip in the complex u plane.

We have examined (Sec. V) Landau's criterion for the stability of a plasma, namely the existence of zeros of $\mathfrak{L}(s)=k^2\omega_p{}^2-\int g_0'(u)(u-s)^{-1}du$ in the closed upper half-plane; we have used a definition of stability different from Landau's, namely that not only should the voltage produced by the disturbance remain bounded, but the disturbance $g_1(u,t)$ in the distribution function of the electrons should remain small in the sense that $\int|g_1(u,t)|\,du$ remains bounded. We have shown that stability depends on the smoothness of the initial disturbances $g_1(u,0)$ which we permit. If we restrict ourselves, as did Landau, to disturbances analytic in a strip $|\Im u|\leq a$ in the complex u plane, then when $\mathfrak{L}(s)$ has zeros with $\Im s>0$, or multiple zeros with $\Im s=0$, $g_0(u)$ is certainly unstable. When $\mathfrak{L}(s)$ has no zeros with $\Im s>0$ and only simple zeros with $\Im s=0$, then, with certain added smoothness conditions on g_0 and integrability conditions on $g_1(u,0)$, g_0 is stable. If $\mathfrak{L}(s)$ has no zeros with $\Im s\geq0$, and if further $|\mathfrak{L}(s)|$ is bounded below when $\Im s>0$, then we need assume only that $g_0'(u)$ and $g_1(u,0)$ are integrable and square integrable or that $g_0'(u)$ is integrable and $g_1'(u,0)$ is integrable and bounded in order to prove that $g_0(u)$ is stable. However, if we permit disturbances $g_1(u,0)$ integrable but not square-integrable, even the Maxwell distribution is unstable. And if $\mathfrak{L}(s)$ has a real zero of first order and we permit all integrable, square integrable disturbances, $g_0(u)$ is unstable.

In Sec. IV, we have applied these criteria to several examples. If a w exists such that $(w-u)g_0'(u)>0$ when $u\neq w$, we have shown that, under certain mild conditions of smoothness, $g_0(u)$ is stable to integrable, square integrable disturbances. As a consequence, we have shown that, with a mild smoothness condition, all isotropic, three-dimensional distributions $f_0(\mathbf{q})$ are stable to integrable, square integrable disturbances. In particular, the Maxwell distribution is stable.

An entirely different approach to the initial value problem, Van Kampen's expansion in normal modes, has been examined in Sec. VII. It has been shown that Van Kampen's normal modes with real frequencies are complete only when $g_0(u)$ is stable, and that Van Kampen has implicitly introduced the assumption of stability (which he never makes explicit) by restricting his attention to isotropic, three-dimensional distributions. The modification of Van Kampen's scheme for unstable u is worked out when $\mathfrak{L}(s)$ has only finitely many zeros with $\Im s\geq0$. It is shown that the normal modes (defined as solutions with exponential time dependence) are no longer complete, and that as a result examination of those modes alone can lead to the erroneous conclusion that an unstable $g_0(u)$ is stable.

Finally, in Sec. VIII, we examine the basis for the linearization, namely that $\partial g_1(u,t)/\partial u$ remains negligible in comparison with $g_0'(u)$ if it began so. We find that for sufficiently smooth $g_0(u)$ subjected to sufficiently smooth disturbances $g_1(u,0)$, the linearization is not justified indefinitely; in fact $\partial g_1(u,t)/\partial u$ grows linearly with time at a rate proportional to its initial amplitude. An example shows that this growth is not always so slow as to be negligible in practical problems. In consequence, serious doubt is cast on any positive conclusions about stability obtained from the linear theory.

Nodal Expansions. III. Exact Integral Equations for Particle Correlation Functions*

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The density expansions of the pair distribution function and potential of average force are analyzed topologically in terms of cutting points and bifocal points. The analysis leads to conversion of the expansions into series with cluster integrals involving products of the total correlation functions, $h(\mathbf{r})=g(\mathbf{r})-1$, at finite density, rather than the usual zero-density Ursell f-functions. An integral equation for the pair potential of average force and the pair distribution function is thus obtained. The equation is formally exact and closed in pair space, involving no triplet distributions such as occur in the treatments of Kirkwood and Yvon-Born-Green. Solution of the equation also yields directly the Ornstein-Zernike direct correlation function. Equations for the free energy in terms of the direct correlation function are presented, thus providing a unified and self-consistent treatment of all thermodynamic properties of a many-body system. The relation of the new equation to the Ornstein-Zernike theory of liquids and to phase transitions is discussed. The possibility of derivation for condensed phases is briefly noted. A simple approximation, involving only the convolutory terms in the cluster expansions of correlation functions, is proposed.

1. INTRODUCTION

THE present series of papers deals mainly with the systematic application of the methods of graph theory to the summation of cluster integral series for distribution and thermodynamic functions of classical many-body systems. In the previous publications of this series[1–3] we have obtained highly summed expressions for the pair ("radial") distribution function, free energy, and pressure of fluids. It has been noted[3] that the repeated summation of certain well-defined classes of graphs in the density expansions of the potential of average force and the pair distribution function results, in the limit, in an integral equation which, within a more general framework, permits a formally exact treatment of a many-body system. The present publication deals, in part, with the details of that development. An equivalent formal treatment has recently been published by J. M. J. van Leeuwen, J. Groeneveld, and J. de Boer.[4] However, the main subject of our present publication consists of an attempt at the elucidation of the physical meaning underlying the formal classification of cluster graphs. We emphasize the close connection of our treatment with the Ornstein-Zernike theory of liquids[5] and thus with the problem of phase transitions. Such an elucidation of the precise physical meaning of entire classes of cluster graphs is certainly necessary if the formal theory is to be applied to actual physical models of many-body systems. So far it has been carried out only for sums of the simplest kinds of graphs (chain and ring integrals), both in classical and quantum systems. We hope that the developments in this and in succeeding publications will ultimately lead to an understanding of the meaning and application of the exact theory and of the approximations derived from it.

The classical treatment of the many-body problem involves two main techniques. In the case of gases the prevalent method is that of density expansions (virial expansions), using the cluster integral technique originated by Ursell, and further developed by Mayer and collaborators.[6] This method is rigorous within the limits of superposition of direct pair potentials, and the radius of convergence of a Maclaurin series in number density.[7] In practice, however, already the calculation of the fourth virial coefficient in a density expansion of pressure (and the corresponding coefficients of density expansions of the potential of average force and the pair distribution function[8]) has not proven feasible analytically except in the case of a fluid of hard spheres with no attractive interaction.[9] Thus, density expansions are useful principally for gases at low density, even though there is no evidence to the effect that, in the absence of phase transitions, their radii of convergence do not extend to large values of this parameter.

The work of McMillan and Mayer[10] has shown that the expressions for the coefficients in density expansions of distribution and thermodynamic functions of dis-

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[1] E. Meeron, Phys. Fluids **1**, 139 (1958).

[2] E. Meeron, J. Chem. Phys. **28**, 505 (1958); errata *ibid.* **29**, 444 (1958).

[3] E. Meeron and E. R. Rodemich, Phys. Fluids **1**, 246 (1958).

[4] J. M. J. van Leeuwen, J. Groeneveld, and J. de Boer, Physica **25**, 792 (1959).

[5] L. S. Ornstein and F. Zernike, Proc. Acad. Sci. Amsterdam **17**, 793 (1914); see also L. Goldstein, Ann. Phys. **1**, 33 (1957).

[6] H. D. Ursell, Proc. Cambridge Phil. Soc. **23**, 685 (1927); J. E. Mayer and M. G. Mayer, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1941).

[7] B. Kahn and G. E. Uhlenbeck, Physica **5**, 399 (1938).

[8] The coefficient of the nth power of density in the virial expansion of pressure corresponds to the coefficient of the n-2-nd power of density in the expansions of pair distribution function and potential of average force.

[9] Majumdar, Bull. Calcutta Math. Soc. **21**, 107 (1929); B. R. A. Nijboer and L. van Hove, Phys. Rev. **85**, 777 (1952).

[10] W. G. McMillan and J. E. Mayer, J. Chem. Phys. **13**, 276 (1945).

persed phases have the same form as for gases, if the direct pair potentials appearing in the latter are replaced by the pair potentials of average force *at infinite dilution* of the disperse phase. Thus, the density expansion method is, in principle, applicable to systems such as solutions, impurities, holes in semiconductors, etc. Here, in addition to the difficulty of evaluating the higher coefficients, we are confronted with the fact that the form of the potentials of average force at infinite dilution is not known for most substances. The method, however, has been applied to ionic solutions where a physically plausible form for the pair potentials of average force at infinite dilution is provided by the Coulombic potential combined with the experimentally determined (and temperature dependent) dielectric constant of the solvent.[11] Recently, an elegant application of density expansions to dilute random ferromagnetic systems has been developed by Brout.[12]

The other principal method for determining correlation and thermodynamic functions is due to Kirkwood,[13] Born and Green, and Yvon.[14] The method consists of differentiating the original partition function with respect to a parameter pertaining to a single particle. One then obtains an exact integral or integrodifferential equation which involves both the pair and triplet distribution functions. Since all thermodynamic functions can be calculated when the pair distribution function is known, we could, in principle, derive all the equilibrium properties of our many-body system if we had an exact relation between the triplet and pair distributions, in addition to the integral equation. Such a relation is not known. An approximation which has been widely used, known as the Kirkwood superposition principle,[13] consists of assuming that the triplet distribution is the product of the three pair distributions (or, equivalently, that the triplet potential of average force is the sum of the three corresponding pair potentials). The superposition principle has been shown to be exact to the first order in the coupling parameters of the particles involved.[15] Its application yields the exact second and third virial coefficients in the density expansion of pressure.[16] Beyond that, however, the superposition principle is certainly not exact. Thus, e.g., its use destroys the consistency between the expression for pressure as obtained from the virial theorem and that derived from the compressibility integral.[9,17] An even more serious inconsistency arises from the fact that the superposition approximation destroys the symmetry of the pair distribution function with respect to interchange of the two particles involved, even though such symmetry is demanded by the very definition of that function.

In the present publication we derive an exact integral equation for the pair potential of average force, i.e., for the pair distribution function. The derivation follows from topological analysis of the structure of the cluster coefficients in the density expansions of the potential of average force, pair distribution function, and the Ornstein-Zernike direct correlation function.[5] This analysis is carried out by the methods employed in previous publications,[1–3] employing the fundamental chain and ring summation technique devised by Montroll and Mayer.[18] The resulting rigorous integral equation, while formally closed (i.e., involving only pair distribution functions), contains a term given by an infinite series of finite-density cluster integrals, thus necessitating an approximation of some form. Such an approximation is in fact readily found, and will be discussed in detail in the following paper in this series.[19]

In the next paragraph of this section we describe the notation used throughout this paper. The following section includes a brief description of cluster expansions of potentials of average force, distribution functions, and free energy, and topological analysis of the clusters involved. In the third section we derive and discuss the new integral equation. The Ornstein-Zernike direct correlation function[5] and a new formula for the free energy form the subject of the fourth section. Section 5 is devoted to a general discussion, including the relation of the singularities of the new integral equation to phase transitions, and the derivation[20] of that equation without recourse to Maclaurin series in number density. Such a derivation would extend the validity of the equation to include condensed phases.

In this exposition we deal principally with one-component systems, for the sake of clarity. However, the final equations are readily extended to include multicomponent systems, using the multicomponent notation introduced in a previous publication.[21] These equations are given in the Appendix.

Three-dimensional Fourier transforms of functions dependent on spatial vectors are extensively used in this publication. We denote such transforms by the same symbols as the original functions, except that the "Fourier space" variables, $\mathbf{k}$, $\mathbf{k}_1$, etc., will be used instead of the original vectors $\mathbf{r}$, $\mathbf{r}_1$, $\mathbf{R}$, etc. Thus, in general,

$$G(\mathbf{k})=\int G(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})d\mathbf{r}, \tag{1.1a}$$

$$G(\mathbf{r})=(2\pi)^{-3}\int G(\mathbf{k})\exp(-i\mathbf{k}\cdot\mathbf{r})d\mathbf{k}. \tag{1.1b}$$

[11] J. E. Mayer, J. Chem. Phys. **18**, 1426 (1950); E. Meeron, *ibid.* **26**, 804 (1957); **28**, 630 (1958).
[12] R. Brout, Phys. Rev. **115**, 824 (1959).
[13] J. G. Kirkwood, J. Chem. Phys. **3**, 300 (1935).
[14] J. Yvon, *Actualities Scientifiques et Industrielles* (Herman et Cie, Paris, 1935); M. Born and H. S. Green, Proc. Roy. Soc. (London) **A118**, 10 (1946).
[15] J. G. Kirkwood and J. C. Poirier, J. Phys. Chem. **58**, 591 (1954).
[16] However, see Appendix to reference 1.
[17] Hart, Wallis, and Pode, J. Chem. Phys. **19**, 139 (1951).
[18] E. W. Montroll and J. E. Mayer, J. Chem. Phys. **9**, 626 (1941).
[19] E. Meeron, submitted to Phys. Rev.
[20] E. Meeron (to be published).
[21] E. Meeron, J. Chem. Phys. **27**, 1238 (1957).

Integrals over the coordinate space of a set $\mathbf{n}$ of n particles will be denoted by a single integration sign and a single differential; any function $F(\mathbf{r}_1,\cdots,\mathbf{r}_n)$ of the coordinates of the particles of that set will be denoted by $F(\mathbf{n})$; the set of coordinates $\mathbf{r}_1,\cdots,\mathbf{r}_n$ will be denoted by $(\mathbf{n})$,

$$\int_1\cdots\int_n F(\mathbf{r}_1,\cdots\mathbf{r}_n)d\mathbf{r}_1\cdots d\mathbf{r}_n=\int F(\mathbf{n})d(\mathbf{n}). \quad (1.2)$$

Since we are dealing with a single component system, in general we omit subscripts on functions pertaining to a definite set of particles. When such identification is necessary, we use the notation $W_{ik}(\mathbf{R}_{ik})$ and $W(ik)$, etc., interchangeably, according to circumstances. The multicomponent notation[21] will be used in the appropriate equations.

2. DENSITY CLUSTER EXPANSIONS OF DISTRIBUTION FUNCTION AND FREE ENERGY

The pair ("radial") distribution function $g(\mathbf{r}_i,\mathbf{r}_j)=g(ij)$ of particles i and j is usually defined by the statement that $\rho^2 g(ij)$ is the probability density of finding particles i and j at the set of coordinates $(ij)=\mathbf{r}_i,\mathbf{r}_j$, in an infinite system at average number density ρ. In a translation-invariant system (e.g., in the absence of external fields), the pair distribution function depends only on the relative coordinates of the two particles: $g(ij)=g(\mathbf{r}_{ij})=g(\mathbf{R})$.

Potentials of average force may be defined in many ways.[22] For our purposes, the most convenient definition of the pair potential of average force is

$$W(ij)=W(\mathbf{R})=-kT\ln g(\mathbf{R}), \quad (2.1)$$

where k is the Boltzmann constant and T is absolute temperature. In a system at zero density, containing only the two particles i and j, the potential of average force reduces to the direct pair potential $U(ij)=U(\mathbf{R})$ and the pair distribution function reduces to the well-known Boltzmann factor. It is therefore convenient to write

$$W(\mathbf{R})=U(\mathbf{R})-kT\epsilon(\mathbf{R};\rho) \quad (2.2)$$

and

$$g(\mathbf{R})=[\exp-\beta W(\mathbf{R})]=\exp[-\beta U(\mathbf{R})+\epsilon(\mathbf{R};\rho)]$$
$$=\exp[-\beta U(\mathbf{R})]\gamma(\mathbf{R};\rho), \quad (2.3)$$

where $\beta=1/kT$. These definitions effect a separation between the density-independent, direct components of $g(\mathbf{R})$ and $W(\mathbf{R})$, and the density-dependent, indirect functions $\gamma(\mathbf{R};\rho)$ and $\epsilon(\mathbf{R};\rho)$, respectively. Obviously, we have $\epsilon(\mathbf{R};0)=0$ and $\gamma(\mathbf{R};0)=1$.

For one-component systems, Mayer and Montroll[23] have proved important combinatory theorems concerning the structure of coefficients in the density expansions of $\epsilon(\mathbf{R};\rho)$ and $\gamma(\mathbf{R};\rho)$. We have

$$\gamma(\mathbf{R};\rho)=1+\sum_{n\geq 1}\frac{\rho^n}{n!}\int P(ij;\mathbf{n})d(\mathbf{n}). \quad (2.4)$$

The integrands $P(ij;\mathbf{n})$ are products of the Ursell

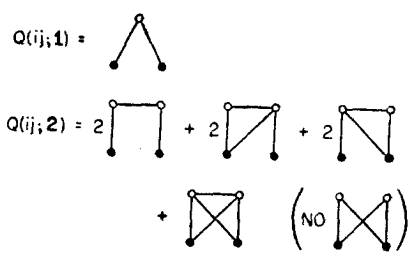

FIG. 2. Examples of products in $Q(ij;\mathbf{n})$.

f-functions,

$$f(lm)=\exp[-\beta U(lm)]-1, \quad (2.5)$$

of pairs of particles l and m belonging to the set $ij+\mathbf{n}$. These products are defined in terms of the topological connections among the particles of this set. We represent each particle by a small circle (node), and each f-function containing the coordinates of a given pair of particles by a line connecting the corresponding pair of nodes. The two particles are then said to be directly connected. A pair of nodes may also be indirectly connected, through one or more intermediate nodes; such connections can be made by one or several paths. When a node is connected to another node by at least two paths, either directly or through mutually exclusive sets of intermediate nodes, the pair is said to be *multiply connected*.[24] A node connected to a set $\mathbf{a}$ of two or more other nodes, either directly or by paths involving mutually exclusive sets of intermediate nodes,[24] is said to be *independently connected* to the nodes of the set $\mathbf{a}$. The integrands $P(ij;\mathbf{n})$, called P-sums, are sums of all possible products of f-functions in which each particle of the set $\mathbf{n}$ is connected independently to particles i

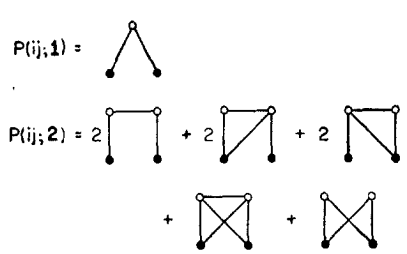

FIG. 1. Examples of graphs in $P(ij;\mathbf{n})$. Numbers before graphs indicate the number of times the corresponding topological type of product of f-bonds appears in the sum, and result from the number of ways in which particles of $\mathbf{n}$ may be distributed among the nodes. Particles i and j are indicated by black dots and particles of n by circles.

[22] See, e.g., T. L. Hill, *Statistical Mechanics* (McGraw-Hill Book Company, Inc., New York, 1956), for a survey.

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

[24] The intermediate nodes may also be connected among themselves.

and j, and particles i and j are not connected directly one to the other. Graphs describing some products in the sums $P(ij;\mathbf{n})$ are given in Fig. 1. It should be noted that these graphs may be regarded as the classical analogs of the *duals*[25] of the diagrams employed by Feynman,[26] and by Lee and Yang.[27] The direct quantum-mechanical analog of our diagrams is provided by the graphs used by Montroll and Ward[28] and by Levine.[29]

The potential function $\epsilon(\mathbf{R},\rho)$ was shown by Mayer and Montroll[23] to be given by

$$\epsilon(\mathbf{R},\rho)=\sum_{n\geq 1}\frac{\rho^n}{n!}\int Q(ij;\mathbf{n})d(\mathbf{n}). \tag{2.6}$$

Here the integrands $Q(ij;\mathbf{n})$ (Q-sums) are sums of all possible products of Mayer f-functions, defined in the same manner as the P-sums, but with the further restriction that nodes of the set $\mathbf{n}$ must now also be connected among themselves independently of nodes i and j, i.e., without involving these nodes. Examples are given in Fig. 2. Equations (2.5) and (2.6) were later extended to multicomponent systems.[21]

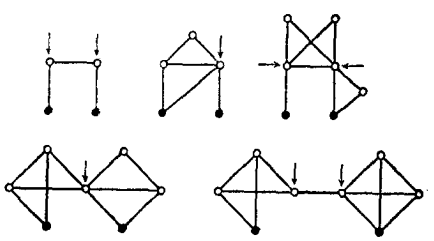

FIG. 3. Examples of products containing cutting points (indicated by arrows). These are the products constituting $\tau(\mathbf{R})$.

The corresponding density expansion for the *coordination energy density* (the Helmholtz free energy of interaction per unit volume) $-\beta F_i V^{-1}$ was obtained for one-component systems by Born and Fuchs,[30] and later extended to multicomponent systems.[31] We have

$$\frac{-\beta F_i}{V}=A(\rho)=\sum_{n\geq 2}\frac{\rho^n}{n!}\int R(\mathbf{n})d(\mathbf{n}), \tag{2.7}$$

where V is the volume. The integrands $R(\mathbf{n})$ here are sums of products of f-functions in which all particles of the set $\mathbf{n}$ are multiply connected. The only exception is $R(\mathbf{2})$ which consists simply of the single f-function $f(ij)$. The integrations are carried out over the coordinates of all particles of the set $\mathbf{n}$, except one, with respect to the coordinates of that one particle.[32] The pressure P is now given by

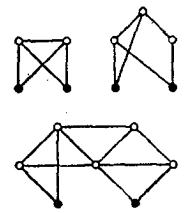

FIG. 4. Graphs with no cutting points. These constitute $\zeta(\mathbf{R})$.

$$\beta P=\rho-\rho\frac{\partial}{\partial\rho}A(\rho)+A(\rho). \tag{2.8}$$

This relation was also extended to multicomponent systems.[21,31] In practice, a more useful quantity is given by the coordination energy per particle

$$-\beta F_i N^{-1}=A(\rho)/\rho=S(\rho). \tag{2.9}$$

The equation for pressure now becomes

$$\beta P=\rho-\rho^2\frac{\partial}{\partial\rho}S(\rho). \tag{2.10}$$

3. THE PROTOTYPE EXPANSION AND THE INTEGRAL EQUATION

After the introductory definitions of Sec. 2, we are ready for more detailed topological analysis of the graphs constituting the Q-sums and P-sums. A little reflection will show that the P-sums are, in effect, products of the Q-sums (Figs. 1 and 2). Therefore, we shall confine the detailed analysis to the Q-sums, and present the final results for $\gamma(\mathbf{R};\rho)$ in terms of $\epsilon(\mathbf{R};\rho)$. First, we note that the graphs belonging to the Q-sums may be divided into two classes. In Fig. 3 we have the first class of the Q-graphs. These are all characterized by the fact that each graph can be separated into two or more graphs by cutting at one or more points. These points of separation are known in graph theory as *cutting points* (or articulation points). On the other hand, we have the second class of graphs, depicted in Fig. 4, which cannot be thus separated into two or more connected graphs. In other words, these graphs contain no cutting points.

We separate the two types of graphs in each Q-sum and put each type in a separate integral. The sum of the integrals of all graphs containing cutting points (with each integral multiplied by the appropriate factor $\rho^n/n!$) is denoted by $\tau(\mathbf{R};\rho)$ and called the τ-sum. It should be emphasized that this sum contains *parts* of each integral of $Q(ij;\mathbf{n})$, $n=1$ to ∞. The corresponding sum of all integrals of graphs containing no cutting points is denoted by $\zeta(\mathbf{R};\rho)$. Clearly, the first term in this ζ-sum starts with $n=2$ (see Fig. 2). Thus,

[25] The dual here is obtained on replacing point by line, and line by point, in the original diagram.
[26] R. P. Feynman, Phys. Rev. **76**, 749, 769 (1949).
[27] T. D. Lee and C. N. Yang, Phys. Rev. **113**, 1165 (1959).
[28] E. W. Montroll and J. C. Ward, Phys. Fluids **1**, 55 (1958).
[29] H. Levine, Phys. Fluids (in press).
[30] M. Born and K. Fuchs, Proc. Roy. Soc. (London) **A166**, 391 (1938).
[31] K. Fuchs, *ibid.* **A179**, 408 (1942).
[32] It should be noted that perhaps the simplest and most generally applicable derivation of the cluster expansion of $A(\rho)$ has been recently devised by Brout (reference 12).

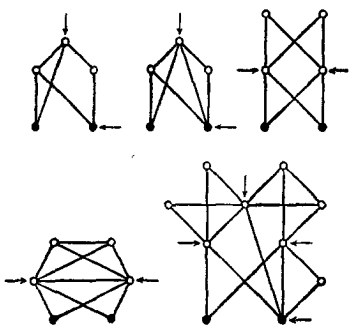

FIG. 5. ζ-graphs containing bifocal points (indicated by arrows).

formally, we may write

$$\epsilon(\mathbf{R},\rho)=\tau(\mathbf{R},\rho)+\zeta(\mathbf{R},\rho). \tag{3.1}$$

Let us now take a look at the τ-sum (Fig. 3). Let us define *adjacent* cutting points by the statement that there are no other cutting points between two such adjacent cutting points (or between a cutting point and node i or j to which it is adjacent). Between such two points there are only subgraphs which contain no cutting points. These subgraphs, however, contain not only graphs from the ζ-sum but also their products, and *products* of graphs from the τ-sum. In addition, each adjacent pair of cutting points may be connected by a direct f-bond. The only type of connection not allowed here is any *single* graph from the τ-sum. Since the nodes in the subset between adjacent cutting points are connected to the rest of the nodes only through these two cutting points, we can integrate over the coordinates of the connecting subset separately, and the integral will be a function only of the relative coordinates of the two adjacent cutting points. From this factorization of the integral it follows that we may sum over all possible subsets between these cutting points, and all allowed combinations of connecting subgraphs. Now, *all* possible connections between the adjacent cutting points, including the direct f-bond, are given by the function

$$h(\mathbf{r};\rho)=[1+f(\mathbf{r})]\gamma(\mathbf{r};\rho)-1=g(\mathbf{r})-1. \tag{3.2}$$

This can be seen as follows. Any two nodes from the set $\mathbf{n}$ (or node i or j and one node from the set $\mathbf{n}$) can be connected by a direct f-bond, by a Q-graph, by a product of Q-graphs, or by a f-bond combined with either of the two previous types of connection. All connections *via* a single Q-graph would thus be given by $\epsilon(\mathbf{r};\rho)$, with $\mathbf{r}$ the vector from one node to the other. Connections *via* a product of s Q-graphs are then given by $[\epsilon(\mathbf{r};\rho)]^s$; this includes all possible combinations of products of different or identical Q-graphs. However, many identical graphs would thus be counted many times over, even though they correspond to the same f-bond product. (Thus, e.g., in $P(ij;2)$, Fig. 1, interchange of the two nodes of the set **2** in the last graph does not result in a new f-bond product). From straightforward combinatory arguments it follows[11] that $[\epsilon(r;\rho)]^s$ has to be divided by $s!$ in order to avoid such a multiple counting of identical f-bond products. Thus, summing over all s from 1 to ∞, we get just $\exp[\epsilon(\mathbf{r};\rho)]-1=\gamma(\mathbf{r};\rho)-1$. This combination does not contain the direct f-bond. Therefore we add $f(\mathbf{r})[\gamma(\mathbf{r};\rho)-1]$, and finally we add the single bond $f(\mathbf{r})$. The sum is just the function $h(\mathbf{r};\rho)$ of Eq. (3.2). This function, however, contains also all single Q-graphs, including those with cutting points, i.e., it contains the entire τ-sum. Since the τ-sum contains cutting points, it has to be excluded from among the allowable subgraphs connecting any two adjacent cutting points. This is done simply by substracting $\tau(\mathbf{r};\rho)$ from the function $h(\mathbf{r};\rho)$ defined in Eq. (3.2). Thus we define the function $c(\mathbf{r};\rho)$ connecting any two adjacent cutting points in the τ-sum by

$$c(\mathbf{r};\rho)=h(\mathbf{r};\rho)-\tau(\mathbf{r};\rho). \tag{3.3}$$

Now, consider the Mth term in $\tau(\mathbf{R})$, containing n cutting points. The integration is over the coordinates of the M particles, and the integral is multiplied by the factor $\rho^M/M!$ The M particles are divided into the n particles constituting the cutting points, and into $n+1$ subsets each of which contains a_m particles, with $1\leq m\leq n+1$. Each subset of a_m particles is located on a graph with a_m nodes and no cutting points. The set $\mathbf{M}$ can be divided into the subsets $\mathbf{n}$ and $\mathbf{a}_m$ in $M!/n!a_1!\cdots a_{n+1}!$ ways. The factor $M!$ is cancelled by the factor $1/M!$ before the integral, and the factors $1/a_m!$, each multiplied by ρ^m (taken from ρ^M), are absorbed into the appropriate terms of the functions $c(\mathbf{r};\rho)$. This leaves the total integral multiplied by $\rho^n/n!$ However, the n cutting points can be distributed in $n!$ ways between particles i and j. Thus, the factor $1/n!$ is cancelled, and we obtain

$$\tau(\mathbf{R};\rho)=\sum_{n\geq 1}\rho^n\int c(i1;\rho)c(12;\rho)\cdots \times c(n-1,n;\rho)c(nj;\rho)d(\mathbf{n}), \tag{3.4}$$

$$c(lm;\rho)=c(\mathbf{r}_{lm};\rho).$$

This equation represents simply a grouping of terms in the τ-sum according to increasing number of cutting points. As we shall see later (Sec. 4), the function $c(\mathbf{r};\rho)$ is just the Ornstein-Zernike direct correlation function.[5]

We now take the Fourier transform of both sides of Eq. (3.4), using the convention of Eq. (1.1). Applying the multiple convolution theorem on Fourier trans-

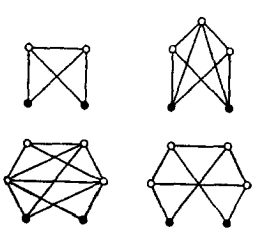

FIG. 6. ζ-graphs with no bifocal points. These are the prototypes.

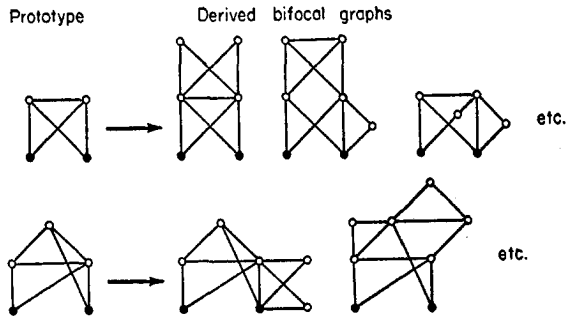

FIG. 7. Derivation of graphs containing bifocal points from prototypes.

forms,[33] we obtain

$$\tau(\mathbf{k};\rho)=\sum_{n\geq 1}\rho^n[c(\mathbf{k};\rho)]^{n+1}=\frac{\rho[c(\mathbf{k};\rho)]^2}{1-\rho c(\mathbf{k};\rho)}. \quad (3.5)$$

By using Eq. (3.3), rearranging, and inverting, we have

$$\tau(\mathbf{R})=\rho\int h(\mathbf{R}-\mathbf{r})[h(\mathbf{r})-\tau(\mathbf{r})]d\mathbf{r}$$
$$=\rho\int h(\mathbf{R}-\mathbf{r})[h(\mathbf{r})-\epsilon(\mathbf{r})+\zeta(\mathbf{r})]d\mathbf{r}. \quad (3.6)$$

In Eq. (3.6) and from now on omit the variable ρ from our functions, their density dependence being implied.[34]

Equation (3.6), on substitution in (3.1), yields

$$\epsilon(\mathbf{R})=\rho\int h(\mathbf{R}-\mathbf{r})[h(\mathbf{r})-\epsilon(\mathbf{r})+\zeta(\mathbf{r})]d\mathbf{r}+\zeta(\mathbf{R}). \quad (3.7)$$

Since $h(\mathbf{r})$ is given in terms of $\epsilon(\mathbf{r})$ [Eqs. (3.2) and (2.3)], we have here an integral equation involving two unknown functions, and we must express one in terms of the other. In order to do this, let us take a closer look at the graphs included in $\zeta(\mathbf{R})$. We note that these graphs can be again classified into two groups. In Fig. 5 we have some ζ-graphs which are characterized by the fact that each of these can be separated into two or more graphs by cutting at one or more *pairs* of nodes. Each of the resulting separate graphs contains at least one node, and *nodes i and j must remain in the same graph.* The pairs of nodes at which separation of the original graph is effected will be called *field bifocal points*, or, briefly, bifocal points.[35] In Fig. 6 we have some ζ-graphs which contain no such bifocal points. These ζ-graphs will be called *prototypes*. We now note that any graph of the first group (containing bifocal points) is derived from a prototype on replacing the direct f-bond in the prototype by the appropriate subgraph (Fig. 7). Clearly, all these possible subgraphs are included in the function $h(\mathbf{r})$. Thus, the ζ-sum may be contracted as follows:

$$\zeta(\mathbf{R})=\sum_{n\geq 2}\frac{\rho^n}{n!}\int Z(ij;\mathbf{n})d(\mathbf{n}). \quad (3.8)$$

Here the integrands $Z(ij;\mathbf{n})$ are sums of all possible products of functions $h(\mathbf{r})$ connecting the particles of the set $ij+\mathbf{n}$ in protype patterns. In Fig. 8 we have the graphs describing $Z(ij;2)$ and $Z(ij;3)$.

Equations (3.7) and (3.8) provide, in principle, a set of equations closed in pair space whose solution would yield values for the pair potential of average force $W(\mathbf{R})$, the pair distribution function $g(\mathbf{R})$, the total correlation function $h(\mathbf{R})$, and the direct correlation function $c(\mathbf{R})$. Of course, their practical application is limited by the fact that $\zeta(\mathbf{R})$, Eq. (3.8), is an infinite series of highly connected cluster integrals. Further discussion of Eqs. (3.7) and (3.8) is postponed to the last section. However, we would like to note here that, within the limits of validity of density expansions, these equations are exact.

The prototype expansion of the pair distribution function is now readily obtained from Eqs. (2.3).

$$g(\mathbf{R})=\exp[-\beta U(\mathbf{R})+\tau(\mathbf{R})]$$
$$\times\left[1+\sum_{n\geq 2}\frac{\rho^n}{n!}\int H(ij;\mathbf{n})d(\mathbf{n})\right], \quad (3.9)$$

with $\tau(\mathbf{R})$ given by Eq. (3.6). The sums $H(ij;\mathbf{n})$ are sums of all possible products of graphs of $Z(ij;\mathbf{m})$, derivable within the set $ij+\mathbf{n}$. Thus, we have $H(ij;2)=Z(ij;2)$, $H(ij;3)=Z(ij;3)$, but $H(ij;4)=Z(ij;4)+4[Z(ij;2)]^2$.

A comparison of the prototype expansions with the original Mayer-Ursell cluster expansions may be of interest. Instead of the direct pair potentials $U(\mathbf{r})$ in the density expansions, we have the pair potentials of

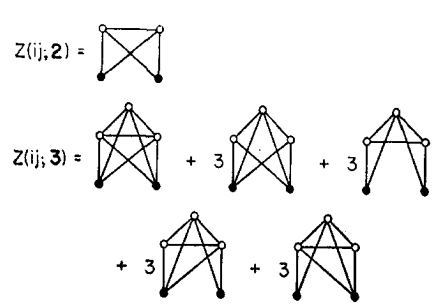

FIG. 8. Graphs describing $Z(ij;2)$ and $Z(ij;3)$ in the prototype expansion.

[33] A general derivation is given in the Appendix to the third reference in footnote 11. The theorem was first published by Montroll and Mayer (reference 18).

[34] Strictly speaking, the present derivation of Eq. (3.6) is valid only for $|\rho c(\mathbf{k})|<1$. When $|\rho c(\mathbf{k})|\geq 1$, Eq. (3.5) is an analytic continuation for $\tau(\mathbf{k})$. However, this analytic continuation is justified by the fact that the equivalence of Eqs. (3.4) and (3.6) is easily proven by induction.

[35] The definition of a (general) bifocal point would not involve the restriction on nodes i and j to remain in the same graph. We omit the prefix "field" throughout the present paper for the sake of brevity. Trifocal points and focal points of higher order can be defined in an entirely analogous manner. A cutting point now becomes a (general) unifocal point.

average force in the prototype expansions, and a large number of graphs included in density expansions is missing from prototype expansions. It should be emphasized that the bonds in prototype expansions are density dependent. Finally, we would like to note that the prototype expansions seem to represent a complete summation of the density cluster expansions. Any further summation of prototype graphs would necessitate analytic methods for evaluation of n-polar integrals (as opposed to the relatively simple bipolar integrals employed in convolutions). Such techniques do not appear to be available at present. Furthermore, the combinatory problems involved are quite formidable.

The derivation of the corresponding prototype expansion for the coordination energy density is considerably more complicated. This derivation forms one of the subjects of the next paper in this series.[19]

4. THE DIRECT CORRELATION FUNCTION AND THE ORNSTEIN-ZERNIKE INTEGRAL EQUATION

As we have mentioned in the previous section, the function $c(\mathbf{R})$ is the direct correlation function first defined by Ornstein and Zernike.[5,36] As is well known, the function $h(\mathbf{R})=g(\mathbf{R})-1$ correlates total density fluctuations at the two points separated by $\mathbf{R}$, including also the effects of indirect correlations through all the remaining particles of the system. This interpretation can be seen from the following considerations. The *average* density around a particle j when particle i is fixed at $\mathbf{R}=\mathbf{r}_{ij}$ is given by $\rho g(\mathbf{R})$. However, the average density in the system is ρ. Thus, the mean density fluctuation around j, due to the presence of particle i is given by $\rho g(\mathbf{R})-\rho=\rho h(\mathbf{R})$. The physical meaning of the direct correlation $c(\mathbf{R})$ is not quite as simple. However, the function is mathematically clearly defined by the Ornstein-Zernike integral equation

$$h(\mathbf{R})=c(\mathbf{R})+\rho\int h(\mathbf{R}-\mathbf{r})c(\mathbf{r})d\mathbf{r}. \tag{4.1}$$

Equation (4.1) expresses the fact that the *total* correlation $h(\mathbf{R})$ in density fluctuations is the sum of the *direct* correlations $c(\mathbf{r})$ from all points in the system. From this interpretation it is seen[5] that the direct correlation function $c(\mathbf{R})$ is finite and of short range even at critical points.

We now proceed to outline the proof that the direct correlation function is indeed given by the relation (3.3). The density expansion of $c(\mathbf{R})$ may be written as a Maclaurin series,

$$c(\mathbf{R})=\sum_{n\geq 0}\frac{\rho^n}{n!}c_n(\mathbf{R}),\quad c_n(\mathbf{R})=\left[\frac{\partial^n c(\mathbf{R})}{\partial\rho^n}\right]_{\rho=0}. \tag{4.2}$$

[36] In the original publication, Ornstein and Zernike use the symbol $f(\mathbf{r})$ to denote $\rho c(\mathbf{r})$, and the symbol $g(\mathbf{r})$ to denote $\rho h(\mathbf{r})$. The present notation is adopted in order to avoid confusion with the usual symbols for the pair distribution function and the Ursell f-function.

Now, Eq. (3.3) means that each coefficient in the density expansion of $c(\mathbf{R})$ includes only those graphs from the corresponding coefficient in the expansion of $h(\mathbf{R})$ which contain no cutting points. On letting $\rho=0$ in Eq. (4.1), we obtain

$$c_0(\mathbf{R})=h_0(\mathbf{R})=f(\mathbf{R}). \tag{4.3}$$

On differentiating Eq. (4.1) once with respect to ρ, letting $\rho=0$, and rearranging, we obtain

$$c_1(\mathbf{R})=h_1(\mathbf{R})-\int h_0(\mathbf{R}-\mathbf{r})c_0(\mathbf{r})d\mathbf{r}$$

$$=h_1(\mathbf{R})-\int f(\mathbf{R}-\mathbf{r})f(\mathbf{r})d\mathbf{r}. \tag{4.4}$$

But from the density expansion of $g(\mathbf{R})$, Eqs. (2.3) and (2.4), and the definition $h(\mathbf{R})=g(\mathbf{R})-1$, it follows that

$$h_1(\mathbf{R})=\exp[-\beta U(\mathbf{R})]\int P(ij;1)d\mathbf{r}_1$$

$$=[1+f(\mathbf{R})]\int f(\mathbf{R}-\mathbf{r})f(\mathbf{r})d\mathbf{r}. \tag{4.5}$$

Equations (4.5) and (4.4) yield

$$c_1(\mathbf{R})=\int f(\mathbf{R})f(\mathbf{R}-\mathbf{r})f(\mathbf{r})d\mathbf{r}. \tag{4.6}$$

The graph corresponding to this expression (triangle with i, j, and 1 as vertices) has no cutting point. Thus, our statement is true for the zeroth and first terms in the density expansion of $c(\mathbf{R})$. Its extension to include any term in the expansion follows readily by induction, through n-fold differentiation of Eq. (4.1). Since the function $\tau(\mathbf{R})$ in Eq. (3.3) contains all terms in $h(\mathbf{R})$ which have cutting points, and is substracted from $h(\mathbf{R})$, we see that the function $c(\mathbf{R})$ defined by that equation is indeed the direct correlation function as defined by Eq. (4.1). The function $\tau(\mathbf{R})$ may thus be interpreted as the *indirect* correlation function, $\tau(\mathbf{R})=h(\mathbf{R})$ (total correlation)$-c(\mathbf{R})$ (direct correlation). It is immediately seen that Eq. (3.6), the integral equation for $\tau(\mathbf{R})$, is in fact entirely equivalent to the Ornstein-Zernike integral equation, Eq. (4.1).

For the purposes of discussion (Sec. 5), it is convenient to rewrite Eq. (4.1) as follows:

$$h(\mathbf{R})=c(\mathbf{R})+\sum_{n\geq 1}\rho^n\int c(il)c(12)\cdots c(nj)d(\mathbf{n}). \tag{4.7}$$

This equation is obtained from Eq. (4.1) by repeated substitutions. It emphasizes the meaning of the direct correlation function: the total correlation of particles i and j is the sum of the direct correlation, direct correlation through one particle, through two particles, and

so on. The inverse of Eq. (4.7) is

$$c(\mathbf{R})=h(\mathbf{R})+\sum_{n\geq 1}(-\rho)^n\int h(il)h(12)\cdots h(nj)d(\mathbf{n}). \quad (4.8)$$

Further discussion is postponed to Sec. 5.

The isothermal compressibility of our system is given by a formula also derived by Ornstein and Zernike,[5]

$$\frac{1}{K_p}=\beta\frac{\partial P}{\partial\rho}=\left[1+\rho\int h(\mathbf{R})d\mathbf{R}\right]^{-1}=[1+\rho h(\mathbf{k}=0)]^{-1}$$

$$=1-\rho\int c(\mathbf{R})d\mathbf{R}=1-\rho c(\mathbf{k}=0). \quad (4.9)$$

This relation, using standard thermodynamic formulas,[37] results in a new expression for the coordination energy density $A(\rho)$, and thus for the Helmholtz free energy,

$$\partial^2 A(\rho)/\partial\rho^2=c(\mathbf{k}=0). \quad (4.10)$$

Since both $A(\rho)$ and $\partial A(\rho)/\partial\rho$ are zero at $\rho=0$, Eq. (4.10) can be immediately integrated, yielding

$$-\beta F_i V^{-1}=A(\rho)=\int_0^\rho\int_0^{\rho'}c(\rho'';\mathbf{k}=0)d\rho''d\rho'. \quad (4.11)$$

In fact, it appears that the direct correlation function is considerably more convenient in this respect than the customarily employed pair distribution function $g(\mathbf{R})$; the use of $g(\mathbf{R})$ necessitates either its knowledge as a function of a coupling parameter[13] or rather elaborate equations.[38] It should be also noted that Eq. (4.11), coupled with the density cluster expansion of $c(\mathbf{R})$, Eq. (4.2), immediately yields the corresponding expansion of $A(\rho)$, Eq. (2.7). Thus, we see that our integral equation, Eq. (3.7), yields all the thermodynamic quantities of interest in a self-contained and consistent manner.

5. DISCUSSION

As we have noted previously, Eq. (3.7), together with the prototype expansion for $\zeta(\mathbf{R})$, Eq. (3.8), constitutes an exact integral equation for the function $\epsilon(\mathbf{R})$, and thus, through Eq. (2.2), for the pair potential of average force and all other functions derived from it, in particular the direct correlation function $c(\mathbf{R})$ and the pair distribution function, $g(\mathbf{R})$. Several problems arise in connection with the new integral equation. First, we have derived this equation starting from Maclaurin series in number density. Therefore, the integral equation applies only to gases and disperse phases (solutions, impurities, etc.) above their critical temperatures. The radii of convergence of density expansions in the absence of phase transitions are not known. Of course, in the case of distribution functions as functions of activity z, it has been shown[39] that in the absence of phase transitions of any order, all singlet, pair, triplet$\cdots$ distribution functions, and all their derivatives with respect to the activity are continuous in that variable. Therefore, since number density ρ is simply the singlet distribution, it is continuous and continuously differentiable with respect to the activity z as long as we have no phase transition of first order. Hence, the above conclusions regarding the behavior of distribution functions as functions of z apply to them also as functions of ρ. It follows that, in the absence of phase transitions, distribution and related functions have no poles on the positive ρ axis. Therefore, there exists an unique analytic continuation for $h(\mathbf{R})$, $c(\mathbf{R})$, and $W(\mathbf{R})$ beyond the radii of convergence of density expansions. Thus, we may say that our summations are carried out for values of ρ smaller than the radii of convergence of the corresponding density expansions and, since the functions involved must be analytic with respect to number density, the sums which we have obtained [i.e., the integral equation (3.7) and the prototype expansion (3.8)] will be the unique analytic continuations of the original expansions for values of ρ larger than their radii of convergence. This argument holds also if the functions involved have a finite number of complex poles. It breaks down if the complex singularities are infinitely dense, approaching the positive real ρ axis. It appears, however, that such a situation would correspond to a phase transition,[40] and we have excluded this explicitly. Actually, we could not then even require our functions to be continuous and continuously differentiable.[39] We would like to emphasize that our argument applies also to fluids below their critical temperatures. In that case, the analytic continuation of our density expansions should remain valid up to the point of condensation, if indeed such a continuation should be necessary at all (that is, if the radius of convergence of the density expansions is lower than the density of condensation).

From the above considerations it appears that the singularities of Eq. (3.7) would correspond to phase transitions. The fact that $g(\mathbf{R})$ [and, therefore, $h(\mathbf{R})$] is discontinuous as a function of ρ across a first- or second-order phase transition means simply that $h(\mathbf{R})$ will have a different analytic form for each of the phases. On the other hand, the Ornstein-Zernike integral equation (4.1) in Fourier representation is

$$h(\mathbf{k})=\frac{c(\mathbf{k})}{1-\rho c(\mathbf{k})}. \quad (5.1)$$

From Eq. (5.1) it is evident that the singularities of the Ornstein-Zernike integral equation (4.1) will occur at values of ρ such that $1-\rho c(\mathbf{k})=0$ for at least some

[37] For example, by differentiating Eq. (2.8) with respect to ρ.

[38] J. G. Kirkwood and F. P. Buff, J. Chem. Phys. **19**, 774 (1951); see also F. P. Buff and R. Brout, J. Chem. Phys. **23**, 458 (1955).

[39] J. E. Mayer, J. Chem. Phys. **16**, 665 (1948).

[40] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404, 410 (1952).

values of $\mathbf{k}$; we would expect such a singularity to be a branch point yielding different analytic forms for $h(\mathbf{R})$ for each phase.

Now, our integral equation (3.7) in Fourier representation is

$$\epsilon(\mathbf{k})=\tau(\mathbf{k})+\zeta(\mathbf{k})=\frac{\rho c^2(\mathbf{k})}{1-\rho c(\mathbf{k})}+\zeta(\mathbf{k}). \qquad (5.2)$$

Here again we have singularities when $1-\rho c(\mathbf{k})=0$ unless these are *exactly* cancelled by singularities in $\zeta(\mathbf{k})$. Such a coincidence appears extremely unlikely since the function $\zeta(\mathbf{R})$ consists of nonconvolutory integrals fundamentally different from the simple convolutions constituting $\tau(\mathbf{R})$. A detailed evaluation and development of the above considerations will be published separately.[20]

The question of the validity of our integral equation (3.7) for condensed phases (i.e., beyond the first expected singularity) is of particular interest. We note that the Ornstein-Zernike relation (4.1), and thus also the integral equation for $\tau(\mathbf{R})$, is valid also for condensed phases, as is obvious from its derivation.[5] Now, this is a linear integral equation for $h(\mathbf{R})$ in terms of $c(\mathbf{R})$, of a type amenable to the Fredholm method of solution. We have found[20] that the solution is just the series given in Eq. (4.8), or Eq. (3.4). From the theory of the Fredholm method it follows that these series converge absolutely except for certain values of ρ (presumably corresponding to phase transitions).

As has been mentioned previously, the prototype expansion of $\zeta(\mathbf{R})$, Eq. (3.8), is an infinite series of extremely complicated cluster integrals involving the unknown functions

$$h(\mathbf{r})=\exp[-\beta U(\mathbf{r})+\epsilon(\mathbf{r})]-1$$

which are to be found from the solution. The obvious approximation consists of cutting off the prototype expansion after a few terms. However, even if we include only the first term ($n=2$) in $\zeta(\mathbf{R})$, we obtain an integral equation for $\epsilon(\mathbf{R})$ which, to say the least, is not readily amenable to solution even with a high-speed computer, except possibly for extremely simple (and physically unreasonable) direct interaction potentials. Furthermore, the physical meaning of such an approximation is obscure. A still simpler approximation results from assuming $\zeta(\mathbf{R})=0$. If we denote the resulting approximate functions by the subscript $_c$, we have

$$\epsilon_c(\mathbf{R})=\tau_c(\mathbf{R}),\ h_c(\mathbf{R})=\exp[-\beta U(\mathbf{R})+\tau_c(\mathbf{R})]-1. \qquad (5.3)$$

From Eq. (3.7) it follows that we now have a simple closed (though nonlinear) convolution equation, of the Ornstein-Zernike type, for $\tau_c(\mathbf{R})$:

$$\tau_c(\mathbf{R})=\rho\int h_c(\mathbf{R}-\mathbf{r})[h_c(\mathbf{r})-\tau_c(\mathbf{r})]d\mathbf{r}$$
$$=\rho\int c_c(\mathbf{R}-\mathbf{r})[c_c(\mathbf{r})+\tau_c(\mathbf{r})]d\mathbf{r}. \qquad (5.4)$$

It has been shown[19] that this *convolution approximation* represents the limit of the nodal expansion sequence[3] as their order goes to infinity. Furthermore, the function $\tau_c(\mathbf{R})$ contains all graphs in the exact $\epsilon(\mathbf{R})$ which can be wholly evaluated by repeated convolutions, and only these graphs. Finally, $\tau_c(\mathbf{R})$ includes *all* terms in the exact potential of average force which conform rigorously and consistently to the Kirkwood superposition principle,[13] and *only* such terms.

A detailed discussion of the convolution approximation and some of its implications, as well as convolution and prototype expansions for the free energy and equation of state is included in the succeeding paper in this series.[19]

In concluding this discussion, we would like to note that the methods employed in this paper and preceding ones[1–3] appear to be applicable to the quantum-mechanical cluster expansions of Montroll and Ward, Lee and Yang, and Levine.[27–29] In particular, the "activity bond" devised by Lee and Yang[27] appears to provide a promising starting point. It should be noted that the Ornstein-Zernike integral equation (4.1) is valid also for quantum-mechanical correlation functions. However, the concept of potential of average force does not apply in these cases.

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APPENDIX. EQUATIONS FOR MULTICOMPONENT SYSTEMS

As we mentioned previously, our results apply also to multicomponent systems, using the notation employed in a previous publication,[21] which should be consulted for a more detailed explanation of summation conventions, multivariable differentiation, etc.

For a system composed of s kinds of particles we denote the set of s number densities by the boldface letter $\boldsymbol{\rho}=\rho_1, \rho_2\cdots\rho_s$ and the set $\mathbf{n}$ of particles is always composed of s subsets (sometimes empty), of n_l particles of kind l. We define

$$\boldsymbol{\rho}^{\mathbf{n}}=\rho_1{}^{n_1}\rho_2{}^{n_2}\cdots\rho_s{}^{n_s} \qquad (A.1)$$

and

$$\mathbf{n}!=n_1!n_2!\cdots n_s!. \qquad (A.2)$$

All our coordinate-space equations (i.e., equations not involving Fourier transforms) can now be written for multicomponent systems simply by replacing ρ by $\boldsymbol{\rho}$, and n by $\mathbf{n}$. In particular, we have the equivalent of Eq. (3.4),

$$\tau(ij)=\sum_{\mathbf{n}\geq 1}\boldsymbol{\rho}^{\mathbf{n}}\int[\sum_{\text{perm}}c(i\mathbf{1})c(\mathbf{12})\cdots c(\mathbf{n}j)]d(\mathbf{n}). \qquad (A.3)$$

Here the symbol $\sum_{\text{perm}}$ means that we take the sum of the different products of functions $c(lm)$ resulting from all the possible divisions of the set $\mathbf{n}$ of n particles of s kinds, but without considering permutations of particles of the same kind among themselves. On the other hand, Eq. (3.6) now becomes

$$\tau(ij)=\tau_{ij}(\mathbf{R})$$

$$=\sum_{l=1}^{s}\rho_l\int h_{il}(\mathbf{R}-\mathbf{r})[h_{lj}(\mathbf{r})-\tau_{lj}(\mathbf{r})]d\mathbf{r}. \quad \text{(A.4)}$$

This equation is easily shown, by induction (using repeated multivariable differentiations[21]), to be equivalent to Eq. (A.3). The considerations which led to Eq. (3.8) can be taken over, practically word for word, to multicomponent systems. Thus we have

$$\zeta(ij)=\sum_{n\geq 2}\frac{\varrho^n}{n!}\int Z(ij;\mathbf{n})d(\mathbf{n}), \quad \text{(A.5)}$$

and hence

$$\epsilon(ij)=\epsilon_{ij}(\mathbf{R})=\sum_{l=1}^{s}\rho_l\int h_{il}(\mathbf{R}-\mathbf{r})$$

$$\times[h_{lj}(\mathbf{r})-\epsilon_{lj}(\mathbf{r})+\zeta_{lj}(\mathbf{r})]d\mathbf{r}+\zeta(ij), \quad \text{(A.6)}$$

with $h(lm)=\exp[-\beta U(lm)+\epsilon(lm)]-1$. This is the multicomponent analog of Eq. (3.7). By putting $\zeta(ij)=0$, we obtain the convolution approximation for multicomponent systems.

Combinatorial Aspects of the Ising Model for Ferromagnetism. I. A Conjecture of Feynman on Paths and Graphs*

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An identity on paths in planar graphs conjectured by Feynman [H] is rigorously established. This permits a complete analysis of the combinatorial approach to the two-dimensional Ising model with nearest neighbor interaction and 0 external magnetic field previously heuristically discussed by Kac and Ward [KW] and Potts and Ward [PW]. Relevant identities are established for the two-dimensional Ising model with next nearest neighbor interactions and 0 external magnetic field, for the two-dimensional Ising model with nearest neighbor interactions and positive external magnetic field, and for the three-dimensional Ising model with nearest neighbor interactions and 0 external field. For the case of a square net with an odd number of spin locations with nearest neighbor interactions and external field equal to $i\pi/2$, it is shown that the partition function is identically zero for both plane and torus imbedding contrary to a result announced by Lee and Yang [LY; Eq. (48)], which turns out to be correct only for an even number of spin locations.

INTRODUCTION

THE Ising [I][1] model is a mathematical model which has interpretations for (1) ferromagnetism; (2) statistical mechanics of a lattice gas (see Yang and Lee [YL][2] and Lee and Yang [LY][3]); (3) binary substitutional alloys (see Newell and Montroll [NM],[4] pp. 382–383); and (4) adsorption of gases in surfaces ([NM], p. 354). The model has lent itself to exact solutions for some cases, and has reflected such physical phenomena as spontaneous magnetization (see Yang [Y][5]) and the phase transition from gas to liquid phase [YL] [LY]. One important use of the model is that approximate methods for the study of systems of interacting particles are tried out on this model and compared with the exact solution before being applied to more complicated systems.

The two major approaches to the problem as discussed in the review article by Newell and Montroll are (1) the matrix, Lie algebra, and spinor approach of Onsager, Kaufman, and van der Waerden ([NM] pp. 368–373), and (2) the combinatorial approach of van der Waerden and Kac-Ward [KW][6] ([NM], pp. 362–367). The first approach has yielded the solution for $n=2$, nearest neighbor interaction (different for horizontal and vertical neighbors), and zero-magnetic field.

The second approach was formulated by van der Waerden as the problem of finding the number of admissible (each node abuts on an even number of arcs) graphs of length ℓ in the lattice graph formed by decomposing a torus into $\mathfrak{N}^*$ congruent squares and heuristically solved by Kac-Ward to yield results consistent with Onsager-Kaufman [OK].[7] A counterexample[8] to a "topological theorem" used by Kac and Ward is given in the sequel. Newell and Montroll ([NM], pp. 362–367) give a clear account of [KW] with the approximate verdict of a very interesting paper but with theories not yet proven. Potts and Ward [PW][9] in the spirit of [KW] have shown that the latters determinantal approach agrees with Onsager-Kaufman, not merely up to negligible terms depending on boundary effects, but exactly. Feynman, in unpublished work which reached the author by way of Harary [H][10] and oral communication from M. Cohen, has distilled the essence of [KW] getting rid of the enormous determinantal identity, which had heuristic value for [KW], and broke the problem neatly into (1) a conjectured identity (stated as an unsolved problem in [H], p. 10) between a function of weighted paths and the desired function of admissible subgraphs, and, on the assumption of an affirmative resolution of the conjecture, (2) a system of difference equations, reminiscent of random walks, which is solved simply to yield results consistent with Onsager-Kaufman and Kac-Ward.

SUMMARY

In this paper Feynman's conjectured identity between a function of weighted paths and the desired function of admissible subgraphs is generalized to any reasonable planar graph and shown to be correct. A correct identity

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[1] [I] E. Ising, Z. Physik **31**, 253–258 (1925).

[2] [YL] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404–409 (1952).

[3] [LY] T. D. Lee and C. N. Yang, Phys. Rev. **87**, 410–419 (1952).

[4] [NM] G. F. Newell and E. W. Montroll, Revs. Modern Phys. **25**, 353–389 (1953).

[5] [Y] C. N. Yang, Phys. Rev. **85**, 808–816 (1952).

[6] [KW] M. Kac and J. C. Ward, Phys. Rev. **88**, 1332–1337 (1952).

[7] [OK] L. Onsager and B. Kaufman, Phys. Rev. **76**, 1244–1252 (1949).

[8] M. Kac informed the author that M. Cohen had anticipated this counterexample with one somewhat more complicated. At this point the author would like to acknowledge several useful conversations in which M. Cohen acquainted the author with the "state of the art" in the combinatorial approach to the Ising model and found the flaw in an early attempt to disprove Feynman's conjecture.

[9] [PW] R. B. Potts and J. C. Ward, Progr. Theoret. Phys. **13**, 38–46 (1955).

[10] [H] F. Harary, "Feynman's simplification of the Kac-Ward treatment of the two-dimensional Ising problem" (planographed) a chapter in a forthcoming book on graph theory, June 12, 1958.

is given for the torus imbedding using ideas suggested by [PW]. From these results the [KW] determinantal identity and the [PW] determinantal identity are proved to be correct for any reasonable graph imbedded in the plane and torus, respectively. Moreover, for the as yet unsolved cases of next nearest neighbor interaction for dimension two and nearest neighbor interaction for dimension three, identities are established between a class of functions of weighted paths and the desired function of admissible subgraphs, this despite an unpublished result of Kac-Ward (presented with proof here), which indicates that in dimension three no satisfactory system of weights is possible. The difficulty is overcome by assigning weights not to the paths in 3 space, but to their projections in a 2-space. This was suggested by the notion of a knot diagram [A],[16] which comes up in knot theory. It might be remarked that the proof of Feynman's conjecture yielded a novel proposition on the circular arrangement of coins. The conjecture itself yields a curious proposition in free groups (not presented here).

As regards step (2), Feynman's analysis is simplified by employing a notion which Temperly [T][13] used in a slightly different context. This avoids the consideration of the difference equation and its resultant harmonic analysis by directly using the geometrical interpretation of the last part. The relation between Feynman's approach and that of Kac-Ward is roughly the relation between the difference equation analysis of a random walk problem and the transition matrix approach, which arises when the same random walk is presented as a Markov chain. A problem *still unsolved* is effectively carrying out step (2) for the case of next nearest neighbor interactions and the case of dimension three.

For the unsolved case of nonzero external magnetic field, a pair of identities has been developed (only one of which is presented here) between functions of weighted paths and the desired function of admissible subgraphs. In the literature the only concrete result, aside from Yang's result on spontaneous magnetization, on nonzero external magnetic field has been the one stated by Lee and Yang ([LY], p. 417) for the free energy per spin location and the magnetization in the case of external magnetic field equal to $i\pi/2$ in their normalization. It is shown here that for $\mathfrak{N}$, the number of spin locations, odd and $z=-1$, the grand partition function $Z(z=-1;\mathfrak{N}$ odd) is zero and so

$$\lim_{\mathfrak{N}\to\infty} F(z=-1;\mathfrak{N}) = \lim_{\mathfrak{N}\to\infty} 1/\mathfrak{N} \log Z(z=-1;\mathfrak{N})$$

is meaningless. The expression given for

$$\lim_{\mathfrak{N}\to\infty} F(z=-1;\mathfrak{N})$$

in [LY], p. 417, therefore does not apply for general $\mathfrak{N}$, but only for $\mathfrak{N}$ even. Yang, when apprized of the difficulty for $\mathfrak{N}$ odd, pointed out (oral communication) that what this really meant was that in the spirit of the other parts of [YL] and [LY] the order of limits has to be watched and that the physically significant quantity is $g(\Theta)$, the limiting density of roots of the grand partition function on the unit circle. Thus the discovery that for $\mathfrak{N}$ odd there always is a root for $z=-1$ causes no paradox, although of course the different behavior for $\mathfrak{N}$ odd and even is interesting.

UNDIRECTED GRAPHS

Examples of *undirected graphs* are G_1, G_2, and G_3 in Fig. 1. Formally an undirected graph $G=[P_1,\cdots,P_n; A_1,\cdots,A_a]$ is a 1-complex (see Lefschetz [L],[11] pp. 45–47) whose arcs, or 1-cells, are, for simplicity, the broken line segments (with only a finite number of breaks) $\{A_1,A_2,\cdots,A_a\}$, and whose nodes or 0-cells are the points $\{P_1,P_2,\cdots,P_n\}$. In a graph there are incidence relations so that in G_2, P_1 *abuts on*, or is incident with, A_1 and A_2; P_2 abuts on A_1, A_2, A_3, A_4, and A_5; P_3 abuts on A_3; P_4 abuts on A_4; and P_5 abuts on A_5. A *subgraph* of an undirected graph G is a 1-subcomplex of G, so that in particular $[P_1,P_2; A_1,A_2]$ is a subgraph of $G_2=[P_1,P_2,\cdots,P_5; A_1,A_2,\cdots,A_5]$. By an *admissible graph* is meant a graph each of whose nodes abuts on an even number of arcs of the graph. In more formal terms, an admissible graph is a cycle ([L], p. 51) with integers mod 2 as coefficients. Thus $[P_1,P_2; A_1,A_2]$ is an admissible subgraph of G_2, while $[P_1,P_2,P_3; A_1,A_2,A_3]$ is not an admissible subgraph of G_2. The empty graph is a subgraph of every graph and is admissible. It is convenient to extend the notion of the graph so that an arc with both of its endpoints identical is permitted. Thus,

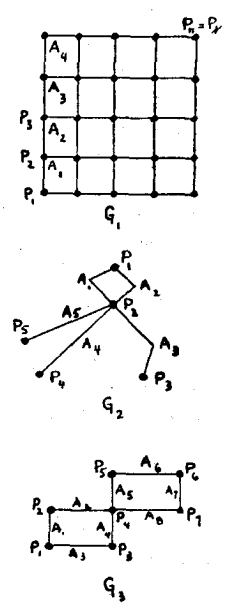


FIG. 1. Undirected graphs.

[11] [L] S. Lefschetz, *Introduction to Topology* (Princeton University Press, Princeton, New Jersey, 1949), p. 45.

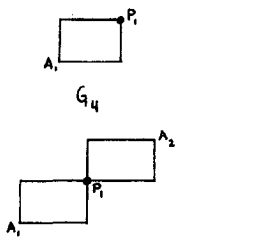


FIG. 2. Arcs whose both endpoints coincide.

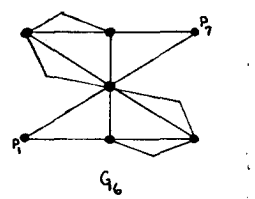


FIG. 3. An admissible nonnormal graph.

in Fig. 2, G_4 and G_5 are graphs. In G_4, P_1 abuts on A_1 twice; and in G_5, P_1 abuts on A_1 twice and on A_2 twice, so that G_4 and G_5 are admissible graphs. A graph is said to be *normal* if it is admissible and each node abuts on not more than four arcs counting multiplicity. Thus G_4 and G_5 are normal, but G_2 is not normal because it is not admissible. In Fig. 3, $G_6=[P_1,\cdots,P_7; A_1,\cdots,A_{14}]$ is admissible but not normal.

DIRECTED GRAPHS

Suppose one has a graph $[P_1,P_2,\cdots,P_n; A_1,\cdots,A_a]$. Associate with each arc A_i a direction so that the arc becomes the *directed arc* D_i going from one abutting node, the tail, to the second abutting node, the head. In Fig. 4, A_1 and A_2 of G_5 have been converted to directed arcs D_1 and D_2, where in both cases the head and tail degenerate into a single node P_1. If the original arc A_i is also associated to the reverse direction, one gets the directed arc D_i^{-1}. If traversal of each of the original arcs in either direction is permitted, then one gets the *directed graph* $[P_1,P_2,\cdots,P_n; D_1,\cdots,D_a,D_1^{-1},\cdots,D_a^{-1}]$. Henceforth, when a graph and its directed graph are mentioned without comment, the directed graph in the last sentence is meant. However, if certain arcs correspond to "one-way streets" then the appropriate directed graph has less than $2a$ directed arcs after the semicolon.

By a *closed path* or *closed directed line sequence* (cdls) is meant a finite, nonempty sequence $D_{i_1}^{\mu_1}D_{i_2}^{\mu_2}\cdots D_{i_s}^{\mu_s}$ of directed arcs ($\mu_i=\pm1$, $1\leq i\leq s$) such that (1) the sequence is considered relative to circular order, so that

$$D_{i_1}^{\mu_1}D_{i_2}^{\mu_2}\cdots D_{i_s}^{\mu_s}=D_{i_2}^{\mu_2}D_{i_3}^{\mu_3}\cdots D_{i_s}^{\mu_s}D_{i_1}^{\mu_1},$$

(2) no two succeeding elements of the sequence are $D_iD_i^{-1}$ or $D_i^{-1}D_i$, $1\leq i\leq a$, and (3) the head of one element of the sequence is identical with the tail of its successor. Since all later paths will be closed, the adjective will be omitted. In Fig. 4, D_1, D_2, D_1D_2, $D_1D_2^{-1}$, D_1^{-1}, D_2^{-1}, and $D_1D_1=D_1^2$ are examples of cdls.

In the same Fig. 4, D_1D_2 and D_2D_1 represent the same cdls; while $D_1D_2D_1^{-1}$ is not acceptable as a cdls. By a nonperiodic cdls is meant one not of the form $(D_{i_1}^{\mu_1}\cdots D_{i_s}^{\mu_s})^r$ for any $r\geq2$.

Henceforth, all the graphs in this paper will be considered imbedded in the plane unless specific mention is made otherwise.

WEIGHTED PATHS (CDLS)

As one traverses a cdls in a path parametrized according to arc length, the angle of the tangent vector should be considered. A question arises when one moves from one line segment to the next as regards the appropriate integral multiple of 2π to use. The rule to be adopted is: choose the integral multiple of 2π so that the difference between the angles of succeeding tangent vectors is in absolute value less than π. This can be made rigorous by using covering spaces (see Griffin [G],[12] [T][13], pp. 270–271).

As one traverses a cdls p, the tangent vector goes through an integral number of revolutions $n(p)$. Let $\bar{W}(p)=-(-1)^{n(p)}$. If $p=D_{i_1}^{\mu_1}D_{i_2}^{\mu_2}\cdots D_{i_s}^{\mu_s}$ and $p^{-1}=D_{i_s}^{-\mu_s}D_{i_{s-1}}^{-\mu_{s-1}}\cdots D_{i_1}^{-\mu_1}$, then $\bar{W}(p)=\bar{W}(p^{-1})$, since $n(p)=-n(p^{-1})$. With each D_i and D_i^{-1} let us associate indeterminate d_i, where the indeterminates commute under multiplication. Thus there are just a indeterminates $d_1, d_2, \cdots, d_a$, not $2a$ indeterminates. With each cdls $p=D_{i_1}^{\mu_1}\cdots D_{i_s}^{\mu_s}$ ($\mu_j=\pm1$; $1\leq j\leq s$), let us associate $W(p)=_{df}\bar{W}(p)d_{i_1}\cdots d_{i_s}$. This is plus or minus a monomial. With each nonperiodic cdls p let us associate its inverse p^{-1} in the same equivalence class $[p]$ and choose one of the two (it does not matter which) as the representative of the equivalence class. Let $I(p)=_{df}I(p^{-1})=_{df}d_{i_1}d_{i_2}\cdots d_{i_s}=_{df}I[p]$. Then $\bar{W}[p]=_{df}\bar{W}(p)=\bar{W}(p^{-1})$ and $W[p]=_{df}\bar{W}(p)I(p)$. As an illustration of the foregoing ideas consider Fig. 4 and Table I. The fact that $W[D_1D_2]+W[D_1D_2^{-1}]=0$ will be referred to as figure eight cancellation.

COUNTEREXAMPLE

Kac and Ward ([KW], p. 1336) state a "topological theorem" which is related to Feynman's conjecture.

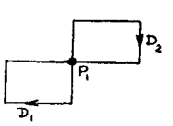


FIG. 4. Directed graph (reverse directions also permitted).

TABLE I. Weighted paths from Fig. 4.

p	$n(p)$	$\bar{W}(p)=\bar{W}(p^{-1})=\bar{W}[p]$	$W[p]=W(p)=W(p^{-1})$
D_1D_2	1	1	d_1d_2
$D_1D_2^{-1}$	0	-1	$-d_1d_2$

[12] [G] J. S. Griffin, Jr., Compositio Mathematica **13**, 270–276 (1958).

[13] [T] H. N. V. Temperley, Phys. Rev. **103**, 1–16 (1956).

This "theorem" ([NM], p. 366) asserts that for a planar, connected, admissible graph G other than a simple closed polygon, the sum of the $\bar{W}(p)$ for all unicursal paths p traversing all of G is zero, where a *unicursal path* traverses each undirected arc only once.

As Kac and Ward point out for G_5 with directed graph of Fig. 4, the paths may be classified as in Fig. 5 and the corresponding reverse paths. It is obvious from Table I that the sum of $\bar{W}(p)$ is zero. The "theorem" is false in general as can be seen from the graph, G_7 of Fig. 6.

Consider three types of behavior at node P_2 as illustrated in Fig. 7. The $\bar{W}(p)$ for the three cases may be tabulated as shown in Table II.

Note that for paths I and II the $\bar{W}(p)$ cancel in pairs so that both the sum of $\bar{W}(p)$ for unicursal paths under I and II are zero. The sum of $\bar{W}(p)$ for the unicursal paths under III is minus four, which gives a contradiction to the "theorem." The correct state of affairs is given by Theorem 1, which is presented in the next paragraph.

FEYNMAN'S CONJECTURE

Let $\Pi^*(1+W[p])$ be the formal infinite product taken over all equivalence classes $[p]$ of nonperiodic cdls. If G_0 is a subgraph $[P_{i_1},P_{i_2},\cdots,P_{i_n};\ A_{j_1},A_{j_2},\cdots,A_{j_a}]$ of graph G, then $\chi(G_0)=_d\Pi_j d_j^{\mu_j}$, where $\mu_j=1$ for $A_j\epsilon G_0$ and $\mu_j=0$ for $A_j\epsilon G_0$. Define G_0 ad G to mean G_0 is an admissible subgraph of G. Let $\sum_{G_0 \text{ ad } G}\chi(G_0)$ be the formal sum of $\chi(G_0)$ taken over all admissible subgraphs G_0 of G, including the empty subgraph.

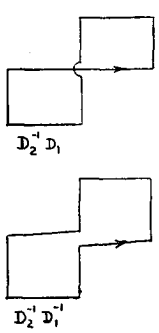


FIG. 5. Two directed graphs associated with G_5.

TABLE II. Weights for unicursal paths traversing all of G_7.

	p	$\bar{W}(p)$	$\Sigma\bar{W}(p)$
I	$D_2D_3^{-1}D_4D_1^{-1}$	+1	
	$D_2D_4^{-1}D_3D_1^{-1}$	−1	
	$D_1D_4^{-1}D_3D_2^{-1}$	1	
	$D_1D_3^{-1}D_4D_2^{-1}$	−1	0
II	$D_2D_4^{-1}D_1D_3^{-1}$	−1	
	$D_2D_1^{-1}D_4D_3^{-1}$	1	
	$D_3D_1^{-1}D_4D_2^{-1}$	−1	
	$D_3D_4^{-1}D_1D_2^{-1}$	1	0
III	$D_2D_1^{-1}D_3D_4^{-1}$	−1	
	$D_2D_3^{-1}D_1D_4^{-1}$	−1	
	$D_4D_3^{-1}D_1D_2^{-1}$	−1	
	$D_4D_1^{-1}D_3D_2^{-1}$	−1	−4

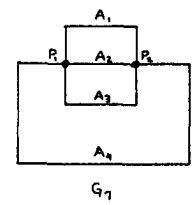
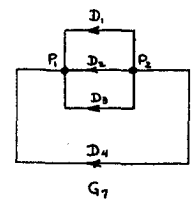
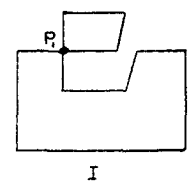
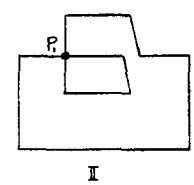


FIG. 6. Counterexample to Kac-Ward.







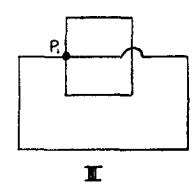


FIG. 7. Classification of unicursal paths on G_7.

Theorem 1. If G is a normal graph, then

$$\Pi^*[1+W(p)]=\sum_{G_0 \text{ ad } G}\chi(G_0). \tag{1}$$

Before launching into the proof of Theorem 1, which is Feynman's conjecture, it should be remarked that for G_1 in Fig. 1, if one sets $d_1=d_2=d_3=\cdots=d_a=z=\tanh K$, then the right-hand side of (1) is the generating function $\sum n(r)z^r$ ([NM], p. 358, Eq. [2.23]) sought in the Ising model (equal horizontal and vertical interactions), where $n(r)$ is the number of admissible subgraphs composed of r arcs. This will be developed much further in the second half of the paper, but one point in this direction will be made now. The information given in the right-hand side is much finer than needed in the Ising model, where all arcs are lumped together as corresponding to equal interaction energy (the indeterminates are set equal to one another) or horizontal arcs are lumped together as corresponding to one interaction energy ("horizontal" indeterminates are set equal to one another) and vertical arcs are lumped together as corresponding to another interaction energy ("vertical"

indeterminates are set equal to one another). As far as the combinatorial end of the problem is concerned, Theorem 1 even handles the case where every nearest neighbor pair of spin locations gives rise to a different size interaction energy.

In order to give the reader an intuitive feeling for the situation being analyzed, some examples are presented. First consider G_4 in Fig. 2 with D_1 being A_1 with a clockwise direction. Here there is just a single nonperiodic cdls equivalence class, namely $[D_1]$. Thus

$$\Pi^*(1+W[p])=1+W[D_1]=1+d_1=\sum_{G_0 \text{ ad } G_4}\chi(G_0).$$

The formal infinite product reduces to a single factor $1+d_1$. The only admissible subgraphs reduce to the empty subgraph and the full graph giving rise to the terms 1 and d_1, respectively. Thus Eq. (1), which is Feynman's conjecture, is trivially verified in this case.

The next simplest case is the nontrivial case of G_5 in Fig. 2. Here, all the essential difficulty in establishing Feynman's conjecture is already present, so the preliminary discussion will not verify the conjecture for that case. This will be left for the proof, but some of the $[p]$ will be considered in order to show that the first few terms in the infinite sum expansion behave properly, and that there is actually an infinite number of factors. Suppose D_i is A_i $(i=1, 2)$ taken in the clockwise direction. Then the results are best presented in tabular form as in Table III. $\Pi^*(1+W[p])=(1+d_1)(1+d_2)(1+d_1d_2)\times(1-d_1d_2)(1-d_1^2d_2)(1+d_1^2d_2)(1-d_2^2d_1)(1+d_2^2d_1)\cdots=(1+d_1+d_2+d_1d_2)(1-d_1^2d_2^2)(1-d_1^4d_2^2)(1-d_2^4d_1^2)\cdots$, which as far as terms of the third order are concerned is $1+d_1+d_2+d_1d_2$. What the proof shows is that as more factors are introduced, the terms $1+d_1+d_2+d_1d_2=\sum_{G_0 \text{ ad } G}\chi(G_0)$ remain while higher degree terms are introduced, ultimately canceling out. In this case one actually gets an infinite number of factors since $\{[D_2],[D_1D_2],[D_1^2D_2],\cdots\}$ constitutes an infinite collection of different nonperiodic cdls equivalence classes.

Proof of Theorem 1. It is immediate that when the left-hand side of (1) is expanded as a formal infinite sum, if G_1 is not an admissible subgraph of G, then the coefficient $\chi(G_1)$ is zero. For the admissible subgraphs a different situation prevails.

First consider the left-hand side of (1) expanded as a sum. Consider certain nodes of order 4, i.e., occurring as head or tail four times, as crossover nodes, e.g., in Fig. 8, consider only such cdls where D_{i1} and D_{i3} only occur in order $D_{i1}D_{i3}$ or $D_{i3}^{-1}D_{i1}^{-1}$, while D_{i2} and D_{i4} only occur in the order $D_{i2}D_{i4}$ or $D_{i4}^{-1}D_{i2}^{-1}$.

TABLE III. Factors in $\Pi^*(1+W[p])$.

$[p]$	$1+W[p]$
$[D_1]$	$1+d_1$
$[D_2]$	$1+d_2$
$[D_1D_2]$	$1+d_1d_2$
$[D_1D_2^{-1}]$	$1-d_1d_2$
$[D_1^2D_2]$	$1-d_1^2d_2$
$[D_1^2D_2^{-1}]$	$1+d_1^2d_2$
$[D_2^2D_1]$	$1-d_2^2d_1$
$[D_2^2D_1^{-1}]$	$1+d_2^2d_1$
...	...

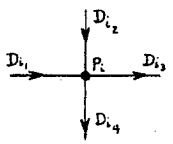
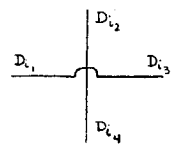


FIG. 8. A crossover node.



Lemma 1. Let G_0 be an admissible subgraph of normal G and $^*\Pi(1+W[p])$ be the product taken over the nonperiodic cdls equivalence classes, where at $n_c(G_0)$ nodes of G_0 a crossover condition is imposed so that all the arcs in the crossover condition are in G_0. Under the circumstance described it is said that G_0 adcc G. When the infinite product is expanded as a sum of monomials in the indeterminates the coefficient of $\chi(G_0)$ is $(-1)^{n_c(G_0)}$.

Proof. Proceed by induction on the number of nodes in G_0. Suppose there is just one node in G_0. There are two possibilities. Either $n_c(G_0)=0$ or $n_c(G_0)=1$. Suppose $n_c(G_0)=0$. Then either G_0 is like G_5 in Fig. 2, or G_0 is like G_4 in Fig. 2. In the first case, by Table III,

$$^*\Pi(1+W[p])=\Pi^*(1+W[p])=(1+d_1)(1+d_2)\times(1+d_1d_2)(1-d_1d_2)\{\Pi^h(1+W[p])\},$$

where $\Pi^h(1+W[p])$ has only factors of the form 1+third or higher order terms in d, and thus $^*\Pi(1+W[p])=1+d_1+d_2+d_1d_2+$higher order terms. Therefore, the coefficient of d_1d_2 is $(-1)^{n_c(G_0)}=(-1)^0=1$ and the lemma is verified for this case. In the second case, G_4 applies and

$$^*\Pi(1+W[p])=\Pi^*(1+W[p])=1+d_1.$$

The coefficient of $\chi(G_0)=d_1$ is 1 and the lemma is verified for this case. Suppose $n_c(G_0)=1$. Now G_5 applies. Then under the same conditions as before

$$^*\Pi(1+W[p])=(1-d_1d_2)\Pi^h(1+W[p])$$

with the same condition on $\Pi^h(1+W[p])$. The coefficient of d_1d_2 is now $(-1)=(-1)^1=(-1)^{n_c(G_0)}$, so that the lemma is verified for this case.

Suppose the proposition is correct for n nodes in $G_0(n>0)$. It is desired to prove it correct for $(n+1)$ nodes. Let $k=n+1-n_c(G_0)$ be the number of free nodes in G_0. Then $0\leq k\leq n+1$. If $k=0$, then all the nodes in G_0 are crossover nodes. The graph with the crossover conditions admits a unique decomposition $\{[p_1],[p_2],\cdots,[p_j]\}$ into path equivalence classes such that $I(p_1)I(p_2)\cdots I(p_j)=\chi(G_0)$. If the decomposition breaks down to one path

equivalence class, then by (see Whitney [W],[14] pp. 281–282) $(-1)^{n_c(G_0)}=\bar{W}[p]$. Thus $*\Pi(1+W[p])=1+(-1)^{n_c(G_0)}\chi(G_0)$, and the lemma follows for this case. If there is more than one path, then by [G] every pair of path equivalence classes in the unique decomposition determines an even number of crossover nodes. Thus when $*\Pi(1+W[p])$ is expanded as a sum, the coefficient of $\chi(G_0)$ is $(-1)^{n_c(G_0)}$.

Institute a proof by induction on k. Suppose $k\geq 1$ and that the proposition is correct for the number of free nodes less than k. Let P be a free node of G_0. Partition the paths of G_0 through P into three classes schematically described by Fig. 9. Let $\mathrm{I(II\ III)}=_{df}\prod_{[p]\in \mathrm{i(ii\ iii)}}(1+W[p])$, where the product is taken over the nonperiodic cdls equivalence classes, which at P show behavior (i ii iii)

$$\mathrm{IV}=_{df}\prod_{[p]\in(\mathrm{i}\cup\mathrm{ii}\cup\mathrm{iii})'}(1+W[p]),$$

where the product is taken over nonperiodic cdls equivalence classes which do not go through P. Thus

$$\Pi^*(1+W[p])=\mathrm{I\ II\ III\ IV}.$$

Suppose $[p]\in$I and $[q]\in$II. Then the product $W[p]W[q]$ has some indeterminate with multiplicity greater than one and can make no contribution to the coefficient of $\chi(G_0)$. Similar examination of II III and I II indicates that when $\Pi^*(1+W[p])$ is expanded as a sum the coefficient of $\chi(G_0)$ is the sum of the corresponding coefficients in I IV; II IV; and III IV.

The contributions to I IV can be regarded as those coming from a graph with one fewer node and with appropriate pairs of arcs incident on that node coalescing, e.g., consider the transition from G_7 in Fig. 6 to Fig. 7. I Analogous remarks are appropriate to II IV; e.g., consider the transition from Fig. 6 to Fig. 7. II By the inductive hypothesis on n, the contributions from I, IV and II IV add to $2(-1)^{n_c(G_0)}$. Consider G_0 as G_0 with P converted from a free node to a crossover node. Then $k-1=n+1-n_c(G_0)-1$ and by the hypothesis of the induction on k the contribution of III IV to the coefficient of $\chi(G_0)$ is $(-1)^{n_c(G_0)+1}$. The total coefficient is therefore $2(-1)^{n_c(G_0)}+(-1)^{1+n_c(G_0)}=(-1)^{n_c(G_0)}$, as was to be proved. This establishes the lemma.

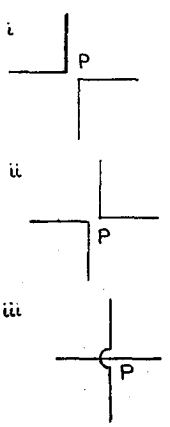


FIG. 9. Possible behavior of path at P.

It must now be shown that when the left-hand side of Eq. (1) is expanded as a formal infinite sum, the remaining coefficients, i.e., the coefficients corresponding to products of indeterminates, where at least one of the exponents is greater than one, are all zero. Thus it must be shown that in the formal infinite sum the coefficient of

$$d_1^{\mu_1}d_2^{\mu_2}\cdots d_a^{\mu_a}=\delta$$

is zero if one of the exponents, say μ_1, is greater than one.

By a path factorization $[pf;\delta]$ of δ is meant a collection $\{[p_1],[p_2],\cdots,[p_k]\}$ of different nonperiodic cdls equivalence classes such that $I[p_1]I[p_2]\cdots I[p_k]=\delta$. It is desired to establish

$$\sum_{[pf;\delta]}(\bar{W}[p_1]\cdots\bar{W}[p_k])=0.$$

It suffices to establish this result for path factorizations, where $I[p_1]$, $I[p_2]$, $\cdots$, $I[p_k]$ all have the common factor d_1. Call such a factorization $[pf;\delta;d_1]$. Let $\{[p_1],[p_2],\cdots,[p_k]\}$ be such a path factorization of type $[pf;\delta;d_1]$. Let $[p_j]$ be represented as $[D_1\alpha_{j1}D_1\alpha_{j2}\cdots D_1\alpha_{jn_j}]$, where (1) D_1 does not occur as a term in α_{j1}, $\cdots$, α_{jn_j}, and (2) D_1^{-1} may occur as a term in α_{j1}, α_{j2}, $\cdots$, α_{jn_j}. Consider $B=\{D_1\alpha_{jr}: 1\leq j\leq k,\ 1\leq r\leq n_j\}$ as the set of building blocks of a $[pf;\delta;d_1]$. Suppose B consists of m_1 equal blocks of a first type, m_2 equal blocks of a second different type, $\cdots$, and m_n equal blocks of the nth different type, where $m_1+m_2+\cdots m_n=n_1+n_2+\cdots n_k=N$. Say then that $B=\{b_1,b_2,\cdots,b_N\}$. Let $[pf;\delta;d_1;B]$ represent the general path factorization of δ using building blocks in B. Note that the building blocks are nonperiodic cdls.

An example of the preceding is $\delta=d_1^2d_2$ for $G=G_5$ with the directions as shown in Fig. 4. The only path factorizations of δ are $\{[D_1D_2],[D_1]\}$, $\{[D_1D_2^{-1}],[D_1]\}$, $\{[D_1^2D_2]\}$ and $\{[D_1^2D_2^{-1}]\}$. Note that $\{[D_1],[D_1],[D_2]\}$ is not a path factorization for δ and that $\{[D_1^{-1}D_2],[D_1]\}$ is the same path factorization as $\{[D_1D_2^{-1}],[D_1]\}$. For $\{[D_1D_2],[D_1]\}$, $B=\{D_1D_2,D_1\}$. For $\{[D_1^2D_2^{-1}]\}$, $B=\{D_1D_2^{-1},D_1\}$.

It is desired to prove

$$\sum_{[pf;\delta;d_1]}(\bar{W}[p_1]\bar{W}[p_2]\cdots)=0. \tag{2}$$

Case 1. Suppose the B associated with $[pf;\delta;d_1]$ consists of just one block $[p_1]=[D_1\alpha]$, where α does not have D_1 as an element. Since δ has d_1^2 as a factor,

$$D_1\alpha=D_1\alpha_1D_1^{-1}\alpha_2,$$

where α_1 has neither D_1 nor D_1^{-1} as an element, and where α_2 may have D_1^{-1} as an element but has no D_1 as an element. Then $[p_2]=[D_1\alpha_1^{-1}D_1^{-1}\alpha_2]$ is a nonperiodic cdls equivalence class not equal to $[p_1]=[D_1\alpha]$ and $\bar{W}[p_1]=-\bar{W}[p_2]$. The contribution to the left-hand side of (2) under case 1 is 0.

[14] [W] H. Whitney, Compositio Mathematica 4, 276 (1937).

Case 2. Suppose B consists of more than one block. In this case one wishes to show that

$$\sum_{[pf;\,\delta;\,d_1;\,B]} (\bar{W}[p_1]\cdots)=0. \tag{3}$$

Note that if $[p_1]\epsilon[pf;\delta;d_1;B]$ and $[p_2]\epsilon[pf;\delta;d_1;B]$ and p_1p_2 is a nonperiodic cdls, then

$$\bar{W}[p_1p_2]=-\bar{W}[p_1]\bar{W}[p_2]. \tag{4}$$

This relation is readily extended to an arbitrary number of factors to give if $[p_j]\epsilon[pf;\delta;d_1;B]$, $1\leq j\leq m$ and $\prod_{j=1}^{m} p_j$ is a nonperiodic cdls, making

$$\bar{W}[\prod_{j=1}^{m} p_j]=(-1)^{m-1}\prod_{j=1}^{m}\bar{W}[p_j]. \tag{5}$$

Associate with each b_i, $1\leq i\leq N$, an indeterminate β_i. Suppose the indeterminates commute under multiplication. Let b represent a nonperiodic sequence of the b_i's taken in its circular rather than its linear order. *Note:* An arbitrary number of any of the b_i may occur in any of these sequences. For example, in the case $n_1=2$, $n_2=3$ one may have $b=b_1b_1b_1b_2b_2b_2b_2$. Let β be the product of indeterminates corresponding to b. By applying the extension of (4), (3) follows for case (2) if it can be shown that

Lemma 2.

$$\Pi^{**}(1-\beta)=1-\beta_1-\beta_2-\cdots-\beta_n, \tag{6}$$

where the product is taken over all different nonperiodic sequences b of $b_i\epsilon B$ as in the foregoing (this is what the first asterisk is intended to denote) and the b are to be taken with respect to circular order (this is what the second asterisk is intended to denote).

Proof. Let $\phi(\beta_1,\cdots,\beta_n;t)=\prod^{**}(1-\beta t)$. Then

$$\sum_{i=1}^{n}\beta_i\frac{\partial}{\partial\beta_i}\ln\phi(\beta_1,\cdots,\beta_n;t)=\sum_{i=1}^{n}\beta_i\frac{\partial}{\partial\beta_i}\sum{}^{**}\ln(1-\beta t)$$

$$=-\sum{}^{**}\frac{t\sigma_\beta\beta}{1-t\beta}=-\sum{}^{**}\sigma_\beta(t\beta+t^2\beta^2+t^3\beta^3+\cdots), \tag{7}$$

where the double asterisk denotes as before an operation, now sum, over all different nonperiodic b, each taken with respect to circular order, and σ_β is the sum of the exponents of all the β_i in β. When $t=1$, the extreme right-hand term in the foregoing is

$$-\sum_{i=1}^{n}\beta_i/1-\sum_{i=1}^{n}\beta_i.$$

Thus

$$\sum_{i=1}^{n}\beta_i\frac{\partial}{\partial\beta_i}\ln\phi(\beta_1,\beta_2,\cdots,\beta_n;t)$$

$$=\sum_{i=1}^{n}\beta_i\frac{\partial}{\partial\beta_i}\ln(1-\beta_1-\beta_2-\cdots-\beta_n).$$

Since the effect of $\sum\beta_i(\partial/\partial\beta_i)$ on a monomial $\beta_1^{\mu_1}\cdots\beta_n^{\mu_n}$ is to send $\beta_1^{\mu_1}\cdots\beta_n^{\mu_n}$ into $(\mu_1+\mu_2+\cdots+\mu_n)\beta_1^{\mu_1}\cdots\beta_n^{\mu_n}$ and $\ln\phi(0,\cdots,0;1)=\ln 1=0$, it follows that $\ln\phi(\beta_1,\cdots,\beta_n;1)=\ln(1-\beta_1-\cdots-\beta_n)$ for β_1, β_2, $\cdots$, β_n sufficiently small. So the lemma is proved and so is the theorem.

COROLLARY ON COIN ARRANGEMENTS

Lemma 2 has a curious corollary in terms of unordered arrangements of coins into circularly ordered sets as follows: Suppose one has a fixed collection of N objects of which m_1 are of one kind, m_2 are of a second kind, $\cdots$, m_n are of the nth kind, e.g., $N(=10)$ coins of which $m_1(=3)$ are pennies, $m_2(=4)$ are nickels, and $m_3(=3)$ are quarters. By a p.o.k. of the N objects one means an exhaustive unordered arrangement of them into k disjoint, nonempty, circularly ordered sets such that (a) no two circular orders are the same and (b) none are periodic. To continue with the example, arrange the 10 coins into $k(=3)$ piles. It does not matter which is the first pile and which is the second pile, etc. No two piles represent the same circular order, e.g., $\{(p,n),(n,p),(p,n,n,q,q,q)\}$ won't do since (p,n) and (n,p) represent the same circular order. One cannot have (p,n,p,n) since this is periodic. Let π_k be the number of p.o.k. of the N objects.

Corollary. For $N>1$, $\pi_1-\pi_2+\pi_3-\cdots+(-1)^{N+1}\pi_N=0$.

Example. Let the collection of $N(=4)$ objects be $\{p,p,n,n\}$ so that $m_1=m_2=2$

$\pi_1=1$, e.g., (p,p,n,n)

$\pi_2=2$, e.g., $\{(p),(p,n,n)\}\{(n),(n,p,p)\}$

$\pi_3=1$, e.g., $\{(p),(n),(p,n)\}$

$\pi_1-\pi_2+\pi_3=1-2+1=0.$

Proof. In Lemma 2 express the left-hand side as a formal infinite sum collecting terms of homogeneous joint degree, i.e., terms where sums of the exponents of the β_{ij} are the same. When these collected terms are compared with the corresponding collected terms on the right-hand side, the corollary follows.

The corollary was actually proved before the lemma. A conversation with E. Grosswald was helpful in proving the corollary. An alternative proof has been devised by A. Selberg.

EXTENSIONS OF EARLIER REMARKS

(1) In formulating the notion of an undirected graph, the requirement of piecewise linearity could have been relaxed to substituting for each of the closures of line segments the range of a smooth homeomorphism, i.e., a function which is a homeomorphism on a closed interval into the plane and which has a continuous nonvanishing derivative throughout the interval. In order for the rest of the definitions to make sense and for the theorem to be true, at no junction (and this may be a node) between successive smooth curves should the tangent

vectors be along the same line but oppositely oriented, i.e., no cusps.

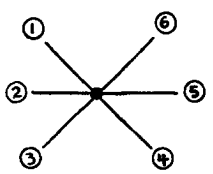
(2) In order to relax the requirement of normality in Theorem 1 it is enough to relax the normality requirement in Lemma 1. To do this one must extend [W], pp. 281–282, and also the argument on p. 206 to the non-normal case. The argument of [W], pp. 281–282, goes through if at each multiple crossover node one looks at the crossovers in pairs and counts each pair in the calculation of N^+ and N^- of [W], pp. 281–282. First examine a node P of order 6 (see Fig. 10).

In considering the contributions to the term in the lemma, classify paths as to which of the other five is immediately contiguous to ①. This classification breaks down into

(a) ① ② (d) ① ⑤
(b) ① ③ (e) ① ⑥,
(c) ① ④

which corresponds to the earlier classification into I, II, and III. Take paths in classification (a); then ① ② can be pulled off the node P as in Fig. 11 without affecting the $W(p)$ of the path or its contribution to the critical

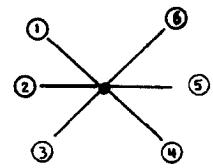
FIG. 10. Node of order 6.



term. By the induction hypothesis the contribution to the coefficient of the critical term from such paths is $(-1)^0$. Consider paths in classification (b). Then ① ③ can be pulled off P as shown in Fig. 12, introducing one crossover node which by the hypothesis of the induction makes a contribution to the critical coefficient of $(-1)^1$. By continuing in this manner one sees that the contribution to the critical coefficient is $(-1)^0+(-1)^1+(-1)^2+(-1)^1+(-1)^0=1$. In the general case where the free node is of "order $2n$" and n is odd, the corresponding sum $2(-1)^0+2(1)^1+\cdots+2(-1)^{n-2}+(-1)^{n-1}=1$. When n is even one gets $2(-1)^0+2(-1)^1+\cdots+2(-1)^{n-2}+(-1)^{n-1}=2-1=1$. Thus the induction proof goes through and the normality hypothesis may be removed from the theorem and the lemma.

(3) In the original Feynman conjecture as formulated in [H], the graphs under consideration are lattice graphs and the counting of the graphs is less detailed. By lattice graphs are meant graphs whose arcs are vertical or horizontal line segments joining all pairs of vertical or horizontal nearest neighbors in a finite, rectangular lattice. If, in the case of lattice graph imbedded in the plane, one sets all indeterminates equal to one another, then the theorem proved provides an affirmative resolution of Feynman's conjecture. If the

FIG. 11. One category of paths at node of order 6.



path imbedded in the torus has no turns, its carrier is an admissible graph not satisfying Feynman's conjecture.

FIRST CROSSOVER THEOREM

The following strengthening of Theorem 1 features the condition (here restated) of Lemma 1 and is useful in the analysis of the Ising model for dimension two with next nearest neighbor interaction ([NM], pp. 354, 374–375) and for dimension three.

Theorem 2. Let G be a normal graph. Let $*\Pi(1+W[p])$ *be the formal infinite product over all different, nonperiodic, cdls equivalence classes, where at k nodes $P_1, P_2, \cdots, P_k$ a crossover condition is imposed, i.e., if the cdls goes through of any the P_i, $1\leq i\leq k$, then the cdls satisfies the crossover condition at P_i. Suppose G_0 adcc G so that G_0 is consistent with the crossover conditions in the sense that if the crossover condition joins two arcs and one of them is in G_0, then the other is in G_0. When the infinite product is expanded as a sum of monomials, the coefficient of $\chi(G_0)$ is $(-1)^{n_c(G_0)}$, where $n_c(G_0)$ is the number of crossover nodes in G_0 such that all the arcs in the crossover condition are in G_0. All the other monomials in the formal infinite sum expansion have coefficient zero.*

To summarize

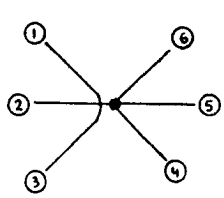
$$*\Pi(1+W[p])=\sum_{G_0 \text{ adcc } G}(-1)^{n_c(G_0)}\chi(G_0).$$

Proof. The coefficient $\chi(G_0)$ for G_0 adcc G has been determined by Lemma 1. The proof that the remaining coefficients are zero follows exactly as in Theorem 1.

TORUS IMBEDDING

Theorems 1 and 2 give combinatorial identities for graphs imbedded in the plane. In Feynman's approach, the identity used is correct for imbedding in the plane, but another stage of his calculation ([H], p. 8, Eq. 11) used imbedding in the torus. Essentially, the correct formula for this case is given in [PW]. What is presented here is a rigorous proof of a generalization of that formula. The extent of the generalization is exactly the same as the extent that Theorem 2 is a generalization of Feynman's conjecture (insofar as it is not limited to

FIG. 12. Another category of paths at node of order 6.



lattice graphs, does not lump all bonds together, and does handle crossover conditions), and the original Kac-Ward identity (for the foregoing reasons and insofar as an infinite number of coefficients, regarding which the Kac-Ward formula says nothing, are shown to be zero).

Consider now an undirected normal graph G on the torus. Take a representation of the torus as a rectangle with edges identified properly. It is required that no node of G be on an edge of the rectangle, that the only points that G have in common with any edge are crossing points, and that G have no points in common with the corners of the rectangle. Let $H(G)$ = number of horizontal edge crossings in G; $V(G)$ = number of vertical edge crossings in G. Note that one horizontal (vertical) edge crossing crosses both identified horizontal (vertical) edges. Let $H(p)$ and $V(p)$ be the corresponding quantities counted with multiplicity for cdls p in G and let

$$W_h(p)=(-1)^{H(p)}W(p) \tag{8}$$

$$W_v(p)=(-1)^{V(p)}W(p) \tag{9}$$

$$W_{h,v}(p)=(-1)^{H(p)+V(p)}W(p). \tag{10}$$

Theorem 3. Let G_0 be an admissible subgraph of a normal G imbedded in a torus, and consider

$$f=\tfrac{1}{2}[{}^*\Pi(1+W_h[p])+{}^*\Pi(1+W_v[p]) +{}^*\Pi(1+W_{h,v}[p])-{}^*\Pi(1+W[p])], \tag{11}$$

where the products are taken over the nonperiodic equivalence classes cdls such that at $n_c(G_0)$ nodes of G_0 a crossover condition is imposed with all the arcs of the crossover condition in G_0. When the infinite product is expanded as a sum of monomials in the indeterminates the coefficient of $\chi(G_0)$ is $(-1)^{n_c(G_0)}$. All the other monomials in the sum have zero coefficients.

Thus

$$f=\sum_{G_0 \text{ adcc } G}(-1)^{n_c(G_0)}\chi(G_0). \tag{12}$$

Suppose G' is a normal graph in the plane formed by appending to G in the complement of the rectangle $H(G)+V(G)$ piecewise linear arcs with no self-intersections, each arc joining a pair of identified points. Consider these new arcs amalgamated with the original arcs, points of which they join. Introduce a node for each intersection of arcs outside the rectangle and require such a node to be a crossover node. To each cdls p of G corresponds a unique cdls p' of G', where

$$W[p']=(-1)^{H(p)+V(p)}W[p]=W_{h,v}[p].$$

G_0' is an admissible subgraph of G' formed by appending $H(G_0)+V(G_0)$ of the previous piecewise linear, non-self-intersecting arcs to G_0, and amalgamating these arcs with the appropriate arcs of G_0. As a consequence of the Jordan Curve Theorem, the number of crossover conditions in G_0' with both sides in G_0' is $n_c(G_0)+H(G_0)V(G_0)$ mod 2. Thus

$${}^*\Pi(1+W_{h,v}[p])={}^*\Pi(1+W[p']) =\sum_{G_0 \text{ adcc } G}(-1)^{n_c(G_0)+H(G_0)V(G_0)}\chi(G_0),$$

$${}^*\Pi(1+W_h[p])=\sum_{G_0 \text{ adcc } G}(-1)^{n_c(G_0)+H(G_0)V(G_0)+V(G_0)}\chi(G_0).$$

The coefficient of $\chi(G_0)$ in f is

$$\tfrac{1}{2}(-1)^{n_c(G_0)+H(G_0)V(G_0)}\{(-1)^{H(G_0)} +(-1)^{V(G_0)}-(-1)^{H(G_0)+V(G_0)}+1\},$$

which for all integral values of $H(G_0)$ and $V(G_0)$ is equal to $(-1)^{n_c(G_0)}$. The other terms in the expansion are equal to zero.

STATUS OF KAC-WARD

Now that Feynman's conjecture relating weighted paths and graphs has been established for the case of plane imbedding and torus imbedding it is in order to look into its precursor, the [KW] determinantal approach. In [KW] it is shown that their determinant gives approximately the right answer for the case of a lattice graph in the torus imbedding. [PW] has given a modification (linear combination of square roots of determinants) which gives exactly the same result as does the algebraic approach of Onsager-Kaufman. What is developed here is a general theorem applying to all graphs (not only lattice graphs) whose validity does not rest on the formulas of Onsager-Kaufman.

For simplicity, consider the case of a plane imbedded graph. For that case Theorem 1 asserts

$$\Pi^*(1+W[p])=\sum_{G_0 \text{ ad } G}\chi(G_0), \tag{13}$$

where the product is taken over different cdls equivalence classes. From this it follows that

$$\Pi^*(1+W(p))=[\sum_{G_0 \text{ ad } G}\chi(G_0)]^2, \tag{14}$$

where the formal infinite product is taken over all different nonperiodic cdls. From (13) it follows that in the expansion of the left-hand side of (14) monomials δ with at least one exponent $\mu_j>2$ have coefficient zero. The Kac-Ward determinant ([KW], pp. 1333–1334) is the sum of all products $W(p)$ for different nonperiodic p, where no two p in a product have the same directed arc in common. If now it can be shown that the sum of all products δ of $W(p)$ (where p is nonperiodic, the maximum μ_j of δ is equal to two, and at least two (p) have the same directed arc in common), is zero, then it follows that for planar graphs G the Kac-Ward determinant is equal to

$$[\sum_{G_0 \text{ ad } G}\chi(G_0)]^2$$

as claimed. Similar to the situation in the latter half of

the proof of Theorem 1, this reduces to showing that for all path factorizations, into paths now instead of path equivalence classes, with just two appearances of the same directed arc, the sum of the products of $W(p)$ is zero. That this sum is zero follows from the fact that if $\alpha_1 \neq \alpha_2$ and $D_1\alpha_1$, $D_1\alpha_2$, $D_1\alpha_1 D_1\alpha_2$ are cdls, then $W(D_1\alpha_1)W(D_1\alpha_2)+W(D_1\alpha_1 D_1\alpha_2)=0$, which is Eq. (4).

If one now expresses the four individual summands of Theorem 3 as square roots of appropriate determinants one justifies the first result in [PW]. The determinantal method which is the major breakthrough in the combinatorial approach has now been justified ([KW], p. 1332; [NM], p. 366). The Feynman conjecture in a certain sense is a deeper proposition than the Kac-Ward identity since it gives the additional information that all higher order terms are zero, although an argument, the one just given, is needed to go from it to the Kac-Ward identity. The Kac-Ward approach has a certain advantage, although in a sense it says less, since it says just enough and that by way of a finite formula rather than by way of a formal sum.

EVALUATION OF PATH FUNCTIONS

Now that Feynman's conjecture has been established for the plane imbedded and torus imbedded cases and the Kac-Ward identity has been established for both cases and some of the relations between them have been clarified, it remains to be seen how these two methods yield the partition function of the Ising problem for the case of a rectangular lattice with different horizontal and vertical interaction constants, the case settled by Onsager and Kaufman. Since the Feynman method has been presented only for the case of both interaction constants the same, in a document [H] not widely circulated, with several approximations made unwittingly (Theorems 1 and 3 were not available when [H] was written), and with the relation to the Kac-Ward method not fully appreciated, it will be presented here in detail, largely following [H], together with a considerable simplification which bypasses the routine harmonic analysis of the difference equation. The simplification stems from an idea used in a different context by Temperley [T].[13] Since the Kac-Ward method is available in widely circulated form [KW], only its connection with the Feynman method will be discussed here.

According to [NM], pp. 358–359, finding the desired partition function leads either via the low-temperature expansion or the high-temperature expansion to finding

$$\sum_{G_0 \text{ ad } G} \chi(G_0),$$

where (1) G is a rectangular graph imbedded in a torus (so that the top and bottom boundaries are identified as well as the extreme left and right boundaries) rather than in a plane for simplicity at the later stages of the calculation, (2) the indeterminates corresponding to horizontal arcs are all set equal to x, and (3) the indeterminates corresponding to vertical arcs are all set equal to y. For this choice of G, if p has k arcs $-W(p) = (-1)^{n(p)}$ is the product of k factors (weights), each of which is acquired in going from one arc in p to the next, following the circular order. There are three alternatives: (1) going straight ahead in which case the factor is one, (2) making a left turn in which case the factor is $\alpha = \exp[i(\pi/4)]$, and (3) making a right turn in which case the factor is $\bar{\alpha}$. What one is doing here is regarding $(-1)^{n(p)}$ as equal to $\exp[(i/2)\int_p \text{curvature } ds]$, expressing the latter in Stieltjes form and allowing for discrete changes in the tangent angle. The effect of introducing weights is that in traversing part of a path p, by multiplying the appropriate weights one can measure the contribution one has made toward $-W(p)$. Feynman's method—as does the Kac-Ward method—capitalizes on these weights. One of the unsuccessful approaches to the three-dimensional problem has been to search for corresponding weights, and a corresponding $W(p)$ for paths on lattice graphs in three dimensions.

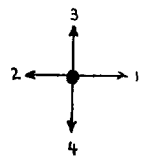


FIG. 13. Notation for direction of steps.

Let (m,n), $0 \leq m \leq M-1$, $0 \leq n \leq N-1$, be the Cartesian coordinates of point of the lattice in the torus. Naturally, there will be no confusion between the use of n for the second coordinate and the earlier use of n for number of nodes. Because of the torus imbedding, when a term is added to the first component it will be modulo M, and when a term is added to the second component it will be modulo N. As a directed path moves along the torus it may go right, (m,n) to $(m+1,n)$; left, (m,n) to $(m-1,n)$; up, (m,n) to $(m,n+1)$; or down, (m,n) to $(m,n-1)$, which directions are indicated in Fig. 13 by 1, 2, 3, or 4.

Let $\beta_{jk}(m,n,r,s)$, $1 \leq j \leq 4$, $1 \leq k \leq 4$, $-\infty < m < \infty$, $-\infty < n < \infty$, $0 \leq r$, $0 \leq s$, be the sum of the weights of all directed paths starting from the origin in direction j, making r horizontal steps and s vertical steps, thus reaching (m,n), and ultimately leaving (m,n) in direction k. Note that $r+s \geq m+n$. Thus the directed path in Fig. 14 contributes $\bar{\alpha}$ to $\beta_{31}(0,1,0,1)$ and makes no contribution to $\beta_{32}(0,1,0,1)$, to $\beta_{33}(0,1,0,1)$, or to $\beta_{34}(0,1,0,1)$. The same directed path contributes $\bar{\alpha}$ to $\beta_{31}(2,0,2,2)$, while it makes no contribution to $\beta_{32}(2,0,2,2)$, to $\beta_{33}(2,0,2,2)$, or to $\beta_{34}(2,0,2,2)$. The contribution it makes to $\beta_{33}(3,0,3,2)$ is 1. It makes no contribution to $\beta_{jk}(m,n,r,s)$ when $j \neq 3$.

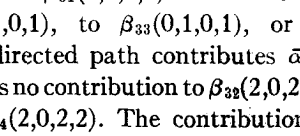


FIG. 14. A directed (nonclosed) path.

Let

$$\beta_{jk}(m,n,0,0)=d_f\delta_{jk}\delta_{m0}\delta_{n0}.$$

Thus

$$\beta_{jk}(0,0,0,0)=d_f\delta_{jk}.$$

Let

$$S(r,s)=d_f\sum_{j=1}^{4}\beta_{jj}(0,0,r,s),$$

which is the sum of the weights of all closed paths starting from the origin and returning to the origin after r horizontal and s vertical steps.

The step leading to any point (m,n) can come from any of the four points $(m-1,n)$, $(m+1,n)$, $(m,n-1)$, or $(m,n+1)$. In order to establish recurrence relations for $\beta_{jk}(m,n,r,s)$, it is convenient to let

$$\begin{aligned}\beta_{j1}&=\beta_{j1}(m-1,n,r-1,s),\\ \beta_{j2}&=\beta_{j2}(m+1,n,r-1,s),\\ \beta_{j3}&=\beta_{j3}(m,n-1,r,s-1),\\ \beta_{j4}&=\beta_{j4}(m,n+1,r,s-1),\\ \mathfrak{B}_j(m,n,r,s)&=(\beta_{j1}(m,n,r,s),\beta_{j2}(m,n,r,s),\cdots).\end{aligned}$$

Thus, for $0\le m\le M-1$, $0\le n\le N-1$,

$$\begin{aligned}\beta_{j1}(m,n,r,s)&=\beta_{j1}+0+\beta_{j3}\bar{\alpha}+\beta_{j4}\alpha,\\ \beta_{j2}(m,n,r,s)&=0+\beta_{j2}+\beta_{j3}\alpha+\beta_{j4}\bar{\alpha},\\ \beta_{j3}(m,n,r,s)&=\beta_{j1}\alpha+\beta_{j2}\bar{\alpha}+\beta_{j3}+0,\\ \beta_{j4}(m,n,r,s)&=\beta_{j1}\bar{\alpha}+\beta_{j2}\alpha+0+\beta_{j4}.\end{aligned}\tag{15}$$

Let

$$\mathbf{B}_j(a,b,r,s)=\frac{1}{MN}\sum_{m=0}^{M-1}\sum_{n=0}^{N-1}\mathfrak{B}_j(m,n,r,s)\times\exp\left[-2\pi i\left(\frac{am}{M}+\frac{bn}{N}\right)\right];$$

then

$$\mathfrak{B}_j(m,n,r,s)=\sum_{a=0}^{M-1}\sum_{b=0}^{N-1}\mathbf{B}_j(a,b,r,s)\exp\left[2\pi i\left(\frac{am}{M}+\frac{bn}{N}\right)\right].$$

Let $B(a,b,r,s)$ be the 4×4 matrix whose jth row is $\mathbf{B}_j(a,b,r,s)$, and let $\beta(m,n,r,s)$ be the analogous 4×4 matrix. Introduce the generating functions

$$\begin{aligned}B(a,b;x,y)&=\sum_{r\ge0,\,s\ge0}B(a,b,r,s)x^ry^s,\\ \beta(m,n;x,y)&=\sum_{r\ge0,\,s\ge0}\beta(m,n,r,s)x^ry^s.\end{aligned}$$

This could be avoided in [H], which considers only equal horizontal and vertical interactions. By a standard calculation (e.g., see Feller[15] [F], Chap. XIV), utilizing the difference equations with initial conditions it follows that

$$B(a,b;x,y)=(I-\mathfrak{M})^{-1}=\sum_{j=0}^{\infty}\mathfrak{M}^j,$$

where I is the 4×4 identity matrix and

$$\mathfrak{M}=\begin{bmatrix}x\beta & 0 & \bar{\alpha}y\gamma & \alpha y\bar{\gamma}\\ 0 & x\bar{\beta} & \alpha y\gamma & \bar{\alpha}y\bar{\gamma}\\ \alpha x\beta & \bar{\alpha}x\bar{\beta} & y\gamma & 0\\ \bar{\alpha}x\beta & \alpha x\bar{\beta} & 0 & y\bar{\gamma}\end{bmatrix}\tag{16}$$

with $\beta=\exp(-2\pi ia/M)$ and $\gamma=\exp(-2\pi ib/N)$. Let $x=Xt$ and $y=Yt$. Then $\mathfrak{M}^n$ is a homogeneous function of degree n in t, and

$$\begin{aligned}&\sum_{\substack{r,s\ge0\\ r+s\ge1}}\frac{B(a,b;r,s)X^rY^s}{r+s}\\ &\qquad=\sum_{j=1}^{\infty}\frac{\mathfrak{M}^j(X,Y)}{j}=-\ln|I-\mathfrak{M}(X,Y)|,\end{aligned}$$

$$\begin{aligned}&\mathrm{Tr}\sum_{\substack{r,s\ge0\\ r+s\ge1}}\frac{\beta(m,n,r,s)x^ry^s}{r+s}\\ &=-\sum_{a=0}^{M-1}\sum_{b=0}^{N-1}\exp\left[2\pi i\left(\frac{ma}{M}+\frac{nb}{N}\right)\right]\mathrm{Tr}\ln|I-\mathfrak{M}|,\end{aligned}\tag{17}$$

$$\mathrm{Tr}\sum_{\substack{r,s\ge0\\ r+s\ge1}}\frac{\beta(0,0,r,s)x^ry^s}{r+s}=-\sum_{a=0}^{M-1}\sum_{b=0}^{N-1}\ln|I-\mathfrak{M}|.$$

By Theorem 1

$$\begin{aligned}\ln\sum_{G_0\text{ ad }G}\chi(G_0)&=\ln\Pi^*(1+W[p])=\ln\Pi^*[1-(-W[p])]\\ &=-\Sigma^*\left[\sum_{j=1}^{\infty}\frac{(-W[p])^j}{j}\right]\\ &=-\tfrac{1}{2}\Sigma^*\left[\sum_{j=1}^{\infty}\frac{(-W(p))^j}{j}\right],\end{aligned}$$

where in the last case the outside sum is over different cdls.

If the imbedding were in a torus instead of a plane the last expression would be equal to

$$-\tfrac{1}{2}\mathfrak{N}\sum_{r+s\ge1}\frac{S(r,s)x^ry^s}{r+s},$$

where $\mathfrak{N}=MN$ is the number of nodes on the lattice graph in the torus. Thus if boundary effects (distinction between plane imbedding and torus imbedding) are ignored, one gets

$$\begin{aligned}\ln\sum_{G_0\text{ ad }G}\chi(G_0)&=-\tfrac{1}{2}\mathfrak{N}\sum_{r+s\ge1}\frac{S(r,s)x^ry^s}{r+s}\\ &=\tfrac{1}{2}\mathfrak{N}\sum_{a=0}^{M-1}\sum_{b=0}^{N-1}\ln|I-\mathfrak{M}|,\end{aligned}\tag{18}$$

[15] [F] W. Feller, *An introduction to Probability Theory and its Applications* (John Wiley & Sons, Inc., New York, 1957), 2nd ed.

which is consistent with [KW], pp. 1336–1337, and [H], p. 18. It is noteworthy that once the respective combinatorial identities are established, then the expositions in [H] and [KW] use essentially the same (in some cases unstated) approximations and reduce to the same manipulation of the matrix $\mathfrak{M}$.

In particular, the Feynman method as presented in [H] starts from a combinatorial identity involving weighted paths and admissible subgraphs imbedded in the plane, then uses an argument (valid for torus imbedding) involving closed weighted paths starting from the origin and continuing for r horizontal and s vertical steps, then goes through a standard difference equation calculation as if the imbedding were in the plane, and finally reduces the answer to an expression in $\mathfrak{M}$. In the presentation here the last transition from torus imbedding to plane imbedding is avoided by staying in the torus. Shortly it will be shown how the lengthy but standard calculation can be avoided by giving a direct interpretation of the final answer, utilizing an idea in [T]. The advantage of the Feynman method is that after his combinatorial identity is established one pushes ahead by standard methods with no tricks needed.

The Kac-Ward method starts from a determinantal identity valid for plane imbedding, but they apply the identity to a graph imbedded in the torus "ignoring boundary effects." The reason for doing this is that the evaluation of the enormous $(4MN\times 4MN)$ determinant can be reduced to an eigenvalue problem which has a neat solution in the case of the graph they chose but which has no known solution for the case of plane imbedding. The eigenvalue problem reduces to consideration of the same matrix $\mathfrak{M}$ as in the other case, so that the two methods are substantially equivalent and involve the same approximations. One way of roughly stating the connection between the methods is that Feynman's method is analogous to the treatment of random walks on the line in [F], Chap. XIV, by way of difference equations, and the Kac-Ward method is analogous to the discussion of random walks on a line in [F], p. 341, example (b), as a Markov chain with minus the identity plus the matrix of their determinant playing the role of the transition matrix. The words "roughly speaking" were used since in the analogy real numbers (probabilities) play the role of complex numbers (weights). To offset the advantage of automatic computation in the Feynman approach it should be mentioned that the determinantal approach has been successful ([PW], pp. 42–45) in handling correlations.

AVOIDANCE OF DIFFERENCE EQUATIONS

The difference equation and its succeeding harmonic analysis can be avoided in Feynman's method if one interprets $\mathfrak{M}'$, the transpose of $\mathfrak{M}$, so that β represents one move to the right, $\bar{\beta}=\beta^{-1}$ represents one move to the left, x represents a horizontal move, γ represents a move up, $\bar{\gamma}=\gamma^{-1}$ represents a move down, and y represents a vertical move. The weights α, $\bar{\alpha}=\alpha^{-1}$, 1, and 0 are associated with turns, as before. Each term in $\mathfrak{M}^n$, say

$$m_{jj}^{(n)}=\sum_{n_1,n_2,n_3,n_4} a_{n_1,n_2,n_3,n_4}\beta^{n_1}\gamma^{n_2}x^{n_3}y^{n_4},$$

may be interpreted as the sum of the weights of those paths that start at a fixed point in direction j, continue for n steps of which n_3 are horizontal and n_4 are vertical so that at the end the net horizontal displacement is n_1 and the net vertical displacement is n_2, and finally leave in direction j. If one applies

$$\sum_{a=0}^{M-1}\sum_{b=0}^{N-1} e^{2\pi i\left(\frac{ma}{M}+\frac{nb}{N}\right)}$$

to $m_{jj}^{(n)}$, one singles out the terms corresponding to closed paths. From this, Eq. (17) follows, and the difference equation with its attendant harmonic analysis can be avoided.

PATH FUNCTIONS IN THE TORUS IMBEDDING

It might be asked how to handle the case of torus imbedding without approximation. Theorem 3 provides the clue. In [PW] this is carried through by the determinantal method where, for example, $*\Pi(1+W_h[p])$ corresponds to the square root of a $4MN\times 4MN$ determinant with the weights of a single row of vertical arcs changed by a factor of (-1) with corresponding changes for $*\Pi(1+W_v[p])$ and $*\Pi(1+W_{h,v}[p])$. These large determinants are neatly evaluated in [PW] to give results which agree exactly with Onsager-Kaufman. If one were to apply the difference equation method to evaluate the terms in Theorem 3, in particular $*\Pi(1+W_h[p])$, there are two courses of action that come up naturally. The first is to multiply by (-1) the weights of the "turns" from those lines mentioned in the foregoing, namely, a fixed row of vertical arcs. As a result, difference equations (15) must be modified for those nodes which abut on this row so that in effect one has a system of linear difference equations with variable coefficients. This makes the analysis awkward, and unfortunately a similar awkwardness in aggravated form arises later for next nearest neighbors in dimension 2, for nonzero external magnetic field in dimension 2, and for dimension 3. The neat factoring of the problem into a four-dimensional one does not seem to go through readily.

The second approach is to multiply the weight of each vertical arc by $\exp-(\pi i/N)$. This is neatly achieved by letting $\gamma=\exp-(\pi i(2b+1)/N)$ instead of $\exp-(2\pi ib/M)$. Let $\mathfrak{M}_h$ be $\mathfrak{M}$ with this new value for γ. Then

$$*\Pi(1+W_h[p])=\prod_{a=0}^{M-1}\prod_{b=0}^{N-1}(|1-\mathfrak{M}_h|)^{\frac{1}{4}}.$$

To get $\mathfrak{M}_v$ retain the original γ, but let

$$\beta=\exp(-\pi i(2a+1)/M).$$

To get $\mathfrak{M}_{h,v}$ use the new β and the new γ. Then for the case of a torus imbedded lattice graph

$$\sum_{G_0 \text{ ad } G}\chi(G_0)=\tfrac{1}{2}\{\prod_{a=0}^{M-1}\prod_{b=0}^{N-1}(|I-\mathfrak{M}_h|)^{\frac{1}{2}}+\prod_{a=0}^{M-1}\prod_{b=0}^{N-1}(|I-\mathfrak{M}_v|)^{\frac{1}{2}}+\prod_{a=0}^{M-1}\prod_{b=0}^{N-1}(|I-\mathfrak{M}_{h,v}|)^{\frac{1}{2}}-\prod_{a=0}^{M-1}\prod_{b=0}^{N-1}(|I-\mathfrak{M}|)^{\frac{1}{2}}\}.$$

If one were to try to handle the torus imbedded case from Theorem 3 bypassing the difference equation, then one might try to handle the expression $^*\Pi(1+W_h[p])$ by multiplying weights of a row of vertical arcs by (-1). The resulting lack of homogeneity from node to node causes difficulty as it did in the difference equation approach. In following the progress of a path in acquiring weights it is no longer sufficient to iterate a 4×4 matrix $\mathfrak{M}$, where the four is associated with the four directions to and four directions from each typical node, because there is no single typical node. One is led to consider a $4MN\times4MN$ matrix $\mathfrak{M}_h$ taking each of the arcs separately. One no longer need include factors like β or γ since they merely constitute a means of telling whether or not weights being counted are associated with closed paths. The $\mathfrak{M}$ which does this trick is minus the identity plus the matrix of the Kac-Ward determinant suitably weighted to take care of the vertical arcs in the distinguished row. Let $T(r,s)$ be the sum of weights of all closed paths involving r horizontal and s vertical steps. Note that if the old weights were used then $T(r,s)=\mathfrak{N}S(r,s)=MNS(r,s)$. Instead of Eqs. (17) and (18), one gets

$$\ln\sum_{G_0 \text{ ad } G}\chi(G_0)=-\tfrac{1}{2}\sum_{r+s\geq1}\frac{T(r,s)x^ry^s}{r+s}=\tfrac{1}{2}\ln|I-\mathfrak{M}_h|.$$

Here one naturally goes from Feynman's conjecture to the original Kac-Ward determinant. If the alternative homogeneous weighting is used on all vertical arcs, then one can reduce the calculation directly to that of a 4×4 determinant.

ISING MODEL FOR DIMENSION THREE AND FOR DIMENSION TWO WITH NEXT NEAREST NEIGHBOR INTERACTION

The success of the strategy of using an identity relating paths and graphs valid for plane imbedded graphs or torus imbedded graphs and then in the case of torus imbedded lattice graphs by any of the methods (determinant, difference equation, or direct) evaluating the resulting expression in paths, suggests that a similar approach be used for the Ising model next nearest neighbor interaction with zero-external magnetic field in dimension two and for the Ising model with only nearest neighbor interaction and zero-external magnetic field in dimension three. First it must be made clear what expression in admissible graphs is sought. Kac has informed the author that he and Ward had proved that in a certain sense for the case of dimension three there is no system of weights like the system which they introduced in dimension two and which gave the identity involving paths and admissible graphs.

Armed with this information, the author presents some examples which show that this is true. Nevertheless, by exploiting the notion of graph with crossover nodes for both the cases of next nearest neighbor interaction and dimension three and using weights, which depend on particular projections in two-dimensional spaces for the case of dimension three, identities with sought-for expressions involving weighted paths on the other side are developed for both cases. Some of the motivations and ideas in this section came from the theory of knots, and it may be that a more intrinsic analysis in this direction may yield interesting results. The identities developed (in the case of dimension three there is an identity involving the sought-for expression in admissible subgraphs on one side and an expression in weighted paths, one for almost each two-dimensional projection—which plays the role of a coordinate system) are new but complex, and the evaluation of the expression in weighted paths has not yet been accomplished. Some results relating Feynman's conjecture to the fundamental group and first homology group of the graph as well as identities applicable to group rings will be presented on another occasion.

Consider the earlier lattice graph, with both diagonals of each elementary two cell included and the midpoint of each elementary two cell included as a crossover node. Thus for each (m,n), $0\leq m\leq M-1$, $0\leq n\leq N-1$, append diagonals of the first kind going from (m,n) to $(m+1,n+1)$ and of the second kind going from (m,n) to $(m-1,n+1)$ getting $2\mathfrak{N}=2MN$ new arcs and also append nodes at $(m+\frac{1}{2},n+\frac{1}{2})$, thus getting $\mathfrak{N}$ new nodes each with a crossover condition. Really to be consistent with previous definitions one should have introduced arcs going from (m,n) to $(m+\frac{1}{2},n+\frac{1}{2})$ and from $(m+\frac{1}{2},n+\frac{1}{2})$ to $(m+1,n+1)$, but the nature of the crossover condition is such that a path which traverses the first arc must traverse the second, and so one amalgamates them. The fact that in the new "graph" two different arcs have common inner points causes no problem. The combinatorial problem to which the next nearest neighbor problem reduces is to find

$$g(x,y,u,v)=\sum n_{1,n_2,n_3,n_4}g_{n_1,n_2,n_3,n_4}x^{n_1}y^{n_2}u^{n_3}v^{n_4},$$

where g_{n_1,n_2,n_3,n_4} is the number of admissible subgraphs consistent with the crossover conditions having n_1 horizontal arcs, n_2 vertical arcs, n_3 diagonal arcs of the first kind, and n_4 diagonal arcs of the second kind. The dimension three nearest neighbor Ising model reduces to finding

$$l(x,y,z)=\sum m_1,m_2,m_3 l_{m_1,m_2,m_3} x^{m_1} y^{m_2} z^{m_3}$$

with l_{m_1,m_2,m_3} equal to the number of admissible subgraphs of the given lattice graph in three dimensions with n_1 arcs parallel to the x axis, n_2 arcs parallel to the y axis, and n_3 arcs parallel to the z axis.

WEIGHTED PATHS IN THREE SPACE

One approach to the dimension three case is to assign weights (elements of a field probably noncommutative) to each turn, these as a result assigning weights to cdls so that Feynman's conjecture with these weights is true. A question arises as to what constitutes a "turn." For dimension two there were three allowed turns S, straight ahead, with weight l; L, left with weight $\alpha=\exp(i\pi/4)$; and R, right with weight $\bar{\alpha}$. Reverse is disallowed or, which amounts to the same thing, given weight 0. Suppose one talks of "turns" from current direction, thus getting five allowed turns: S, straight ahead with weight s; L, left with weight l; R, right with weight r; U, up with weight u; and D, down with weight d, instead of the 30 "turns" one would get if a "turn" were specified by the ordered pair consisting of the incoming direction followed by the outgoing direction. Suppose $s=e$, the identity element of the field. In order that each admissible subgraph of the three-dimensional lattice graph be counted correctly, it must be that the product of the field elements corresponding to turns equals $-e$. What Kac and Ward found (oral communication) is that no such uniform assignment of field elements is possible, no matter what the field. One closed path (unknotted) described by successive turns is DSLLDSLSUULS. Thus $dl^2dlu^2l=-e$. Another is DLLDLL. Thus $dl^2dl^2=-e$, $l^{-1}u^2l=e$, $u^2=e$. A similar argument yields $l^2=d^2=e$. But $-e=dl^2dl^2=d^2=e$, which is a contradiction, thus yielding the Kac-Ward assertion.

A more decisive nonexistence theorem involving assignment of field elements to the 30 "turns" would be desirable. Nevertheless, this is negative evidence as regards the possibility of establishing the identity of a function of weighted paths with the desired function of admissible subgraphs.

SECOND CROSSOVER THEOREM

Consider now the three-dimensional lattice graph G. Take a regular projection P of G into some two-dimensional subspace. By a regular projection P is meant one such that if for each $P_0 \epsilon P(G)$ by $\mu(P_0)$ the multiplicity of P_0 (the number of elements of G mapping onto P_0) is meant, then all but a finite number of elements of $P(G)$ have multiplicity one and the remaining elements having finite multiplicity. There are an infinite number of such regular projections. $P(G_0)$ plays the role of the knot diagram in knot theory (see Alexander [A][16]). The "diagram" of a knot ([A], pp. 276–277) depends on the particular projection, but the Alexander polynomial of the knot doesn't depend on the particular projection and the Alexander polynomial can be computed from the "diagram." It was just these considerations, as well as some of the more intimate details in the knot theory development, which motivated the current theorem. For the three-dimensional Ising problem one is interested in

$$\sum_{G_0 \text{ ad } G} \chi(G_0)$$

with no crossover constraints. With proper identification of indeterminates, this reduces to

$$\sum_{G_0 \text{ adcc } P(G)} \chi(G_0)$$

with proper crossover constraints at those image elements (now nodes) whose multiplicity is greater than one.

Since both the three-dimensional Ising model and the two-dimensional Ising model with next nearest neighbor interactions reduce to evaluations of the type

$$\sum_{G_0 \text{ adcc } G} \chi(G_0),$$

consider Theorem 2. Here Eq. (7)

$$*\Pi(1+W[p])=\sum_{G_0 \text{ adcc } G} (-1)^{n_c(G_0)}\chi(G_0).$$

Moreover, for the G of two-dimensional next nearest neighbor interactions, the approximate result following Eq. (18) is

$$\ln \sum_{G_0 \text{ adcc } G} (-1)^{n_c(G_0)}\chi(G_0)=\tfrac{1}{2}\mathfrak{N}\sum_{a=0}^{M-1}\sum_{b=0}^{N-1}\ln|I-\mathfrak{M}_{nnn}|,$$

where now $\mathfrak{M}_{nnn}$ is an 8×8 matrix. The rows of this matrix correspond to the eight different directions of approach to the typical one of the $\mathfrak{N}$ lattice points, its columns are the same with respect to outgoing directions, and its entries reflect the number of horizontal, vertical, and diagonal steps of both kinds (the net displacement and the weight acquired in turning) in each step. The exact expression appropriate for torus imbedding involves the same linear combination of determinants as in the nearest neighbor interaction, but now one has 8×8 determinants. Thus for

$$\sum_{G_0 \text{ adcc } G} (-1)^{n_c(G_0)}\chi(G_0),$$

not only is an identity available, but also a formula for

[16] [A] J. W. Alexander, Trans. Am. Math. Soc. **30**, 275–306 (1928).

evaluating the resulting function of weighted paths. Unfortunately, what is sought for physical applications is

$$\sum_{G_0 \text{ adcc } G} \chi(G_0).$$

For concreteness, think of the next nearest case where at the center point of each of the elementary two cells a crossover condition is imposed. Then

$$f_{CG}(d) = {}^*\Pi(1+W[p]) = \sum_{G_0 \text{ adcc } G} (-1)^{n_c(G_0)}\chi(G_0),$$

where C is the collection of crossover nodes, and d is a vector whose components correspond to the indeterminates, one component for each indeterminate. For each $P_i \epsilon C$, let d_{2i-1}, d_{2i} correspond to the two diagonals in the crossover condition. If

$$\begin{aligned}
&\Delta_i f_{CG}(d) \\
&= d_j \tfrac{1}{2}\{-f_{CG}(d_1, \cdots, d_{2i-2}, -d_{2i-1}, -d_{2i}, d_{2i+1}, \cdots, d_n) \\
&\quad + f_{CG}(d_1, \cdots, d_{2i-2}, -d_{2i-1}, d_{2i}, d_{2i+1}, \cdots, d_n) \\
&\quad + f_{CG}(d_1, \cdots, d_{2i-2}, d_{2i-1}, -d_{2i}, d_{2i+1}, \cdots, d_n) \\
&\qquad + f_{CG}(d_1, \cdots, d_{2i-2}, d_{2i-1}, d_{2i}, d_{2i+1}, \cdots, d_n)\},
\end{aligned}$$

then $\Delta_i f_{CG}(d)$ is equal to the sum of $(-1)^{n_c(G_0)+1}\chi(G_0)$ for those G_0 adcc G with both arms at P_i in the crossover condition plus the sum of $(-1)^{n_c(G_0)}\chi(G_0)$ for all other G_0 adcc G. The effect of Δ_i on $f_{CG}(d)$ is to eliminate undesired minus signs in the expansion of $f_{CG}(d)$, the signs being those associated with the crossover condition at P_i. From this is deduced

Theorem 4.

$$(\prod_{j \epsilon C} \Delta_j) f_{CG}(d) = \sum_{G_0 \text{ adcc } G} \chi(G_0).$$

This is the identity between a function of weighted paths and the function of admissible subgraphs desired for the two-dimensional Ising model with next nearest neighbor interactions and the three-dimensional Ising model with nearest neighbor interactions.

The reformulation for the torus imbedded case is immediate.

ISING MODEL FOR DIMENSION TWO WITH EXTERNAL MAGNETIC FIELD

By means of the low-temperature expansion the Ising model for dimension two with external magnetic field can be ([NM], pp. 358–359) reduced to finding

$$h(x,y,w) = \sum h_{n_1,n_2,n_3} x^{n_1} y^{n_2} w^{n_3},$$

where h_{n_1,n_2,n_3} is the number of 2 chains mod 2 or, equivalently, unions of elementary two cells whose total area is n_3 and whose interior boundary has n_1 horizontal arcs and n_2 vertical arcs. For the case of torus imbedding, the adjective interior is unnecessary. For the case of plane imbedding, ignore boundary effects by letting

$$h_a(x,y,w) = \sum h_{a,n_1,n_2,n_3} x^{n_1} y^{n_2} w^{n_3},$$

where h_{a,n_1,n_2,n_3} is equal to the number of 2 chains mod 2 whose total area is n_3 and whose full boundary has n_1 horizontal and n_2 vertical arcs.

Suppose one steers a course midway between the complications of the pure plane imbedding and those of the torus imbedding. Consider combinatorial identities appropriate to h_a and therefore appropriate to the approximate plane imbedding. The techniques can be extended to the torus imbedding, but this will not be done here.

A key notion is that of an index of an admissible planar graph relative to a point of the plane. Let $i(Q;G)$ be the index mod 2 of a point Q relative to an admissible linear graph G imbedded in R_2 where $Q_a G$. Take any simple arc going from Q to the point at infinity and intersecting G at a finite number of points, no one of which is a node and all of which are crossing points. If the number of intersections of the arc with G is odd, then $i(Q;G)=1$. If the number of intersections of the arc with G is even, then $i(Q;G)=0$. Since the homotopy of an arc past a node of an admissible graph G does not change the parity of the number of intersections with G, note that $i(Q;G)$ does not depend on the arc chosen. An analogous definition can be given for $i(Q;p)$, where now multiplicity must be taken into account. Consider any $[pf;\chi(G)] = \{[p_1]\cdots[p_k]\}$. Then

$$\prod_{j=1}^{k} (-1)^{i(Q;p_j)} = \exp[i\pi \sum_{j=1}^{k} i(Q;p_j)] = (-1)^{i(Q;G_0)}.$$

From this, one gets the following:

Theorem 5. Let G be a planar graph with a set of $n_c(G)$ crossover conditions. Let Q_j, $1 \leq j \leq a$, be points of the plane not on the graph. With each Q_j associate an indeterminate w_j. Assume the indeterminates commute under multiplication and $w_j^2 = 1$, $1 \leq j \leq A$. Then

$$\begin{aligned}
&{}^*\Pi(1+W[p]w_1^{i(Q_1;p)}\cdots w_A^{i(Q_A;p)}) \\
&\quad = \sum_{G_0 \text{ adcc } G} (-1)^{n_c(G_0)}\chi(G_0) w_1^{i(Q_1;G_0)}\cdots w_A^{i(Q_A;G_0)}.
\end{aligned}$$

Note that in the special case of no crossover conditions and G the two-dimensional lattice, the last expression in Theorem 5 becomes $h_a(x,y,w)$ if (1) the $i(Q_j;G_0)$ are given their 0 or 1 determinations and regarded as ordinary integers, (2) one and only one Q_j is placed in each elementary two cell, say at its center, (3) the indeterminates corresponding to horizontal (vertical) lines are set equal to $x(y)$, and (4) all the w_j are set equal to w. An alternative expression for $h_a(x,y,w)$ has been developed involving the convolution of A expressions, but it will not be presented here.

For the case just discussed, one way of modifying the indeterminates in Theorem 2 so as to get the result of

Theorem 5 would be to draw a horizontal line l_j to the right through each Q_j and for each arc A_i let the new indeterminates be

$$d_i \prod_{j=1}^{A} z_j^{\mu_j},$$

where $\mu_j=1$ if A_i intersects l_j and $\mu_j=0$ if A_i does not intersect l_j. If these are used instead of the indeterminates of Theorem 2, then the special case of Theorem 5 results. There are many alternative ways of modifying the indeterminates so as to achieve the same final result.

ISING MODEL WITH A PARTICULAR EXTERNAL MAGNETIC FIELD

Lee and Yang [LY], in section *VE* of their paper (whose notation and results will be used without explanation) on the connection between condensation in a lattice gas and the Ising model of ferromagnetism, summarize the state of knowledge on a two-dimensional ferromagnetic Ising square lattice in a magnetic field. In addition to the Onsager formula [O][17], [K][18] for the partition function with 0 external magnetic field and Yang's formula for the intensity of spontaneous magnetization at 0 magnetic field, they give for the free energy per spin at $z=-1$, which corresponds to a purely imaginary magnetic field equal to $i\pi/2$,

$$F(z=-1) = -\frac{i\pi}{2}-\frac{kT}{4\pi^2}\int_0^\pi\int_0^\pi \log\{(1-x^2)^2[1+(6-4\cos^2 w - 4\cos^2 w^1)x^2+x^4]\}\,dw\,dw^1 \quad ([LY], \text{Eq. } [48]). \tag{19}$$

They reserve the proof of this formula for a later publication, which to the author's knowledge has not appeared. Nor has anybody else given any results on the case of nonzero external magnetic field which Lee and Yang say ([LY], p. 413) is related to the complete solution of the lattice gas model outside the transition region. In the current communication it is shown

$$F(z=-1;\mathfrak{N}) \xrightarrow[\substack{\mathfrak{N}\to\infty \\ \text{odd}}]{} +\infty$$

so that the foregoing Eq. (48) is incorrect.

The total number of spins in the Ising lattice is

$$\mathfrak{N}=[\uparrow]+[\downarrow].$$

The total energy of the Ising lattice is

$$\begin{aligned} U_I &= H([\downarrow]-[\uparrow])+[\updownarrow]\epsilon \\ &= -H\mathfrak{N}+2H[\downarrow]+[\updownarrow]\epsilon. \end{aligned}$$

The grand partition function

$$Z=\exp\left(\frac{-\mathfrak{N}F}{kT}\right)=\sum\exp\left(\frac{-U_I}{kT}\right)$$

$$=\exp\left(\frac{H\mathfrak{N}}{kT}\right)\sum\exp\left[\frac{-2H[\downarrow]}{kT}\right]\exp\left[\frac{-\epsilon[\updownarrow]}{kT}\right],$$

where the sum is over all two to the $\mathfrak{N}$th spin configurations. With Lee and Yang let

$$z=\exp(-2H/kT)$$
$$x=\exp(-\epsilon/kT)$$

and further let $h(A,l;\mathfrak{N})$ be the number of spin configurations with $A=[\downarrow]$ and $l=[\updownarrow]$. Then

$$Z=\exp\left(\frac{H\mathfrak{N}}{kT}\right)\sum_{A,l} h(A,l;\mathfrak{N})z^A x^l.$$

Since

$$h(A,l;\mathfrak{N})=h(\mathfrak{N}-A,l;\mathfrak{N}),$$

it follows if $\mathfrak{N}$ is odd then

$$\sum_{A \text{ even}} h(A,l;\mathfrak{N})=\sum_{A \text{ odd}} h(A,l;\mathfrak{N}).$$

Thus for $z=-1$ and $\mathfrak{N}$ odd,

$$Z(z=-1;\mathfrak{N})=0 \quad \text{and} \quad F(z=-1;\mathfrak{N})=+\infty,$$

contradicting ([LY], Eq. [48]). The argument just presented applies equally well to plane and torus imbedding.

[17] [O] L. Onsager, Phys. Rev. **65**, 117–149 (1944).
[18] [K] B. Kaufman, Phys. Rev. **76**, 1232–1243 (1949).

Ergodicity Conditions in Quantum Mechanics

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In this paper ergodicity conditions for a quantummechanical system are investigated in the line of thought of recent papers of Bocchieri and Loinger and of authors themselves. More precisely, the averaging $\mathfrak{A}$ over all the initial states used in the paper by Bocchieri and Loinger is here substituted by an averaging $\mathfrak{B}$ over the initial states belonging to a given cell; that is to say, over all the microscopic states corresponding to a given macroscopic state. Restrictions to be imposed on the Hamiltonian in order that relation

$$\sum_{\nu=1}^{N} \frac{\mathfrak{B}(Mu_\nu(t)-s_\nu/S)^2}{s_\nu^2/S^2} \ll 1$$

be satisfied are then looked for. These restrictions could be obtained only in an implicit form.

INTRODUCTION

RECENTLY, Bocchieri and Loinger[1] have given an ergodic theorem which may be expressed by the following relation:

$$\sum_{\nu=1}^{N} \frac{\mathfrak{A}M(u_\nu(t)-s_\nu/S)^2}{s_\nu^2/S^2} < \sum_{\nu=1}^{N} \frac{1}{s_\nu} \ll 1. \quad (1)$$

The notations here are the same as those given by other papers.[1,2] More precisely, the energy shell is supposed to be subdivided into N manifolds (cells) $V_1 \cdots V_N$ spanned by the vectors

$$\omega_{\nu i} (\nu = 1, 2, \cdots N; i = 1, \cdots s_\nu; \sum_{\nu=1}^{N} s_\nu = S).$$

$u_\nu(t)$ denotes the quantummechanical probability that at time t the system is in a state belonging to the manifold V_ν; M denotes the time averaging; and $\mathfrak{A}$ an averaging over the initial states.

A stronger version of this theorem has been given later by the authors of this paper[2] and is expressed by the following relation[3]:

$$P(\vartheta(a,\psi_0) > \bar{\vartheta}) < \exp[-\varkappa(s_{\min} a)^{\frac{1}{3}}] + \varkappa + \log \frac{SN}{\bar{\vartheta}},$$

$$\varkappa \cong 0, 3. \quad (2)$$

Here $\vartheta(a,\psi_0)$ represents the time fraction during which even one of the quantities

$$\Delta_\nu(t) \equiv \frac{(u_\nu(t)-s_\nu/S)^2}{s_\nu^2/S^2}$$

alone, for an initial state ψ_0, is greater than a; $P(\vartheta(a,\psi_0) > \bar{\vartheta})$ represents the probability that ϑ be greater than $\bar{\vartheta}$.

The average $\mathfrak{A}$ in (1) and the probability P in (2) are calculated attributing an equal weight to all the initial states of the energy shell. These theorems state essentially that for the greater part of the time the following relation is very accurately verified:

$$u_\nu(t) = s_\nu/S, \quad (3)$$

with the exception of a set of initial state vectors of very small weight. This result can be obtained on the basis of only two assumptions of a very general character: (a) the system has very many degrees of freedom, i.e., the quantities s_ν are very large, and much larger than N; (b) the time evolution operator is unitary.

The interest of theorems (1) and (2) lies mainly in the fact that they show the importance of the role played by the geometrical structure of the energy shell as regards the laws of statistical mechanics. On the other hand, just because of their generality, these theorems cannot provide any ergodicity condition, i.e., they cannot distinguish the physical systems actually approaching thermodynamic equilibrium. This is essentially caused by the fact that the averaging operation on which they rest does not take into account the selection of a particular class of states connected with the nature of macroscopic observations.

We notice in this regard that the choice of the vectors $\omega_{\nu i}$, by means of which the energy shell is decomposed into cells is not arbitrary, but imposed by the nature of macroscopic observation in the sense that a given macroscopic state must be completely characterized by assigning the cell V_ν to which the state vector of the system belongs.

To say, therefore, that a system exhibits an actual tendency towards a state of equilibrium V_E amounts to saying that if one supposes to have found it in a state V_μ in a certain observation, there is a very great probability of finding it in the state V_E in a successive observation. If the state V_E has a microcanonical probability s_E/S very near to one, i.e., much greater than that of all other states, the system will have the

[1] P. Bocchieri and A. Loinger, Phys. Rev. **114**, 948 (1959).
[2] G. M. Prosperi and A. Scotti, Nuovo cimento **13**, 1007 (1959).
[3] This relation, more suitable for our discussion here, can be deduced from (6) of footnote 2 in a way similar to that used there to derive relation (10) from (5).

foregoing mentioned property only if relation (3) or even the weaker one:

$$Mu_\nu(t)=s_\nu/S \tag{4}$$

is verified, not for the overwhelming majority of the microscopic initial states belonging to the whole energy shell, but for the overwhelming majority of those belonging to each cell V_μ. (If this is the case, obviously, the interpretation of the quantity s_ν/S with $\nu\neq E$ as the probability of a fluctuation towards the state V_ν is also justified.)

One can immediately see that this cannot be inferred from theorems (1) and (2): in fact, on the hypersurface of the initial states corresponding to the whole energy shell, the statistical weight of all the states belonging to one of the manifolds V_μ is actually zero. Consequently, it cannot be excluded that they correspond, completely or even for the greater part, to exceptional configurations. (This is the case, for instance, if a partition of the subdivision into cells exists which is invariant with respect to the time evolution operator). For this reason in this paper, since we abandon the point of view of theorem (2) which would be too difficult in this case, we will substitute the averaging $\mathfrak{A}$ of theorem (1) by an averaging $\mathfrak{B}$ performed over all the initial states belonging to the same cell and look for the conditions which the Hamiltonian must satisfy in order that the following two relations be verified:

$$\mathfrak{B}Mu_\nu(t)\cong s_\nu/S, \tag{5}$$

$$\sum_{\nu=1}^{N}\frac{\mathfrak{B}(Mu_\nu(t)-s_\nu/S)^2}{s_\nu^2/S^2}\ll 1. \tag{6}$$

The following example which is very simple, but particularly significant may conveniently illustrate the considerations of this section [see G. Ludwig, Z. Physik **135**, 483 (1953)]. Let us consider a system S composed of two distinct macroscopic systems S_1 and S_2. To characterize macroscopic observations on S_1 and S_2 we will suppose that the energy ranges have been subdivided in consecutive intervals of equal width $(E_a^{(1)}, E_a^{(1)}+\Delta E^{(1)})$, $(E_a^{(2)}, E_a^{(2)}+\Delta E^{(2)})$, respectively, and that in each energy shell obtained, a system of basis vectors $\{\omega^{(1)}{}_{a_1\nu_1 i_1}\}$, $\{\omega^{(2)}{}_{a_2\nu_2 i_2}\}$ has been introduced. Clearly, every macroscopic observation on the whole system will consist of two independent observations on S_1 and S_2, respectively, so that the macroscopic states of the total system S will be characterized by the energy shells $(E_a, E_a+\Delta E)$ with $\Delta E=\Delta E^{(1)}+\Delta E^{(2)}$ and by the basic vectors

$\omega_{a\nu i}=\omega^{(1)}{}_{a_1\nu_1 i_1}\omega^{(2)}{}_{a_2\nu_2 i_2}$, with a_1 and a_2 such that $E_{a_1}{}^{(1)}+E_{a_2}{}^{(2)}=E_a$.

If S_1 and S_2 are thermally isolated, i.e., there are no energy exchanges, then evidently all the cells corresponding to a given pair of values a_1 and a_2 are invariant submanifolds of the total energy shell. If initially S_1 and S_2 are not already in the equilibrium configuration (equal temperature) they will never exhibit any tendency to approach it. On the other hand, if S_1 and S_2 do interact (thermal contact) one should expect that, under reasonable assumptions on the interaction Hamiltonian, S_1 and S_2 actually tend towards thermodynamic equilibrium.

1. SOME PRELIMINARY RELATIONS

We want to recall here, first of all, some formulas which will be needed in performing the foregoing mentioned average.

Let us consider a normalized vector of a complex q-dimensional manifold spanned by the system of orthonormal vectors $\{\varphi_\rho\}$

$$\psi=\sum_1^q{}_\rho\, c_\rho\varphi_\rho.$$

If we attribute an equal statistical weight to all vectors, the extremities of which lie on the hypersphere of equation $\sum_1^q{}_\rho|c_\rho|^2=1$ (i.e., if we attribute to a certain set of vectors, which corresponds to a certain region of the hypersphere, a statistical weight proportional to the area of that region), we obtain for the average value of the nth power of the quantity

$$u=\sum_1^p{}_\rho\,|c_\rho|^2 \quad (p\leq q),$$

the following expression (due to von Neumann)[4]:

$$\langle u^n\rangle_{\mathrm{av}}=\frac{p(p+1)\cdots(p+n-1)}{q(q+1)\cdots(q+n-1)}.$$

By applying this formula in the cases $p=1$, $n=1$ and $p=1$, $n=2$, we get

$$\langle|c_\rho|^2\rangle_{\mathrm{av}}=\frac{1}{q},\quad \langle|c_\rho|^4\rangle_{\mathrm{av}}=\frac{2}{q(q+1)}.$$

On combining the last result with that of case $p=2$, $n=2$ we obtain then

$$\langle|c_\rho|^2|c_\sigma|^2\rangle_{\mathrm{av}}=\frac{1}{q(q+1)}\quad(\rho\neq\sigma).$$

By making use of the preceding results and of symmetry considerations, we finally have

$$\langle c_\rho c_\sigma{}^*\rangle_{\mathrm{av}}=\frac{1}{q}\delta_{\rho\sigma}, \tag{7'}$$

$$\langle c_\rho c_{\rho'}{}^* c_\sigma{}^* c_{\sigma'}\rangle_{\mathrm{av}}=\frac{\delta_{\rho\rho'}\delta_{\sigma\sigma'}+\delta_{\rho\sigma}\delta_{\rho'\sigma'}}{q(q+1)}\cong\frac{\delta_{\rho\rho'}\delta_{\sigma\sigma'}+\delta_{\rho\sigma}\delta_{\rho'\sigma'}}{q^2}. \tag{7''}$$

[4] J. von Neumann, Z. Physik **57**, 30 (1929), Appendix.

2. ERGODICITY CONDITIONS

(a) *Linear theorem*

Let us suppose $\psi_0 \subset V_\mu$, we may put

$$\psi_0 = \sum_1^{s_\mu}{}_j (\omega_{\mu j}, \psi_0)\omega_{\mu j}; \tag{8}$$

we have then

$$u_\nu(t) = \sum_1^{s_\nu}{}_i \sum_1^{s_\mu}{}_{jj'} (\omega_{\mu j}, \psi_0)^* (\omega_{\mu j'}, \psi_0) \times \left(\omega_{\nu i}, \exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j}\right)^* \times \left(\omega_{\nu i}, \exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j'}\right). \tag{9}$$

On applying (7′) to the manifold V_μ one gets

$$\mathfrak{B}[(\omega_{\mu j}, \psi_0)^* (\omega_{\mu j'}, \psi_0)] = \frac{1}{s_\mu}\delta_{jj'},$$

whence

$$\mathfrak{B}Mu_\nu(t) = \frac{1}{s_\mu}\sum_1^{s_\mu}{}_j M \sum_1^{s_\nu}{}_i \left|\left(\omega_{\nu i}, \exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j}\right)\right|^2,$$

so that (5) will be satisfied if

$$\frac{1}{s_\mu}\sum_1^{s_\mu}{}_j M \sum_1^{s_\nu}{}_i \left|\left(\omega_{\nu i}, \exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j}\right)\right|^2 \cong \frac{s_\nu}{S}. \tag{10}$$

(b) *Quadratic theorem*

If we put

$$L^{(\nu)}{}_{\mu;jj'} \equiv \frac{S}{s_\nu}\sum_1^{s_\nu}{}_i \left\{ M\left[\left(\omega_{\nu i}, \exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j}\right)^* \times \left(\omega_{\nu i}, \exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j'}\right)\right] - \frac{s_\nu}{S}\delta_{jj'}\right\},$$

we may write

$$\frac{(Mu_\nu(t) - s_\nu/S)^2}{s_\nu^2/S^2} = \sum_1^{s_\mu}{}_{jj'} \sum_1^{s_\mu}{}_{kk'} L^{(\nu)}{}_{\mu;jj'} L^{(\nu)}{}_{\mu;kk'}{}^* \times (\omega_{\mu j}, \psi_0)^* (\omega_{\mu j'}, \psi_0) \cdot (\omega_{\mu k}, \psi_0)(\omega_{\mu k'}, \psi_0)^*.$$

Hence, if we make use of (7″), which gives

$$\mathfrak{B}[(\omega_{\mu j}, \psi_0)^* (\omega_{\mu j'}, \psi_0)(\omega_{\mu k}, \psi_0)(\omega_{\mu k'}, \psi_0)^*] \cong \frac{1}{s_\mu^2}(\delta_{jj'}\delta_{kk'} + \delta_{jk}\delta_{j'k'}),$$

we obtain

$$\sum_1^N{}_\nu \frac{\mathfrak{B}(Mu_\nu(t) - s_\nu/S)^2}{s_\nu^2/S^2} \cong \sum_1^N{}_\nu \frac{1}{s_\mu^2}\left(\sum_1^{s_\mu}{}_j L^{(\nu)}{}_{\mu;jj} \sum_1^{s_\mu}{}_k L^{(\nu)}{}_{\mu;kk}{}^* + \sum_1^{s_\mu}{}_{jj'} L^{(\nu)}{}_{\mu;jj'} L^{(\nu)}{}_{\mu;jj'}{}^*\right) = \sum_1^N{}_\nu \frac{1}{s_\mu^2}\left[\left(\sum_1^N{}_j L^{(\nu)}{}_{\mu;jj}\right)^2 + \sum_1^{s_\mu}{}_{jj'} |L^{(\nu)}{}_{\mu;jj'}|^2\right],$$

so that (6) will be satisfied if

$$\sum_1^N{}_\nu \frac{1}{s_\mu^2}\left[\left(\sum_1^{s_\mu}{}_j L^{(\nu)}{}_{\mu;jj}\right)^2 + \sum_1^{s_\mu}{}_{jj'} |L^{(\nu)}{}_{\mu;jj'}|^2\right] \ll 1.$$

A reasonable way of satisfying this condition is to suppose

$$\left|\frac{1}{s_\mu}\sum_1^{s_\mu}{}_j L^{(\nu)}{}_{\mu;jj}\right| \ll \frac{1}{N^{\frac{1}{2}}}, \quad \frac{1}{s_\mu^2}\sum_1^{s_\mu}{}_{jj'} |L^{(\nu)}{}_{\mu;jj'}|^2 \ll \frac{1}{N}.$$

That is, explicitly

$$\left|\frac{1}{s_\mu}\sum_1^{s_\mu}{}_j M \sum_1^{s_\nu}{}_i \left|\left(\omega_{\nu i}, \exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j}\right)\right|^2 - s_\nu/S\right| \ll \frac{1}{N^{\frac{1}{2}}}\frac{s_\nu}{S}, \tag{10′}$$

$$\frac{1}{s_\mu}\sum_1^{s_\mu}{}_j \frac{1}{s_\mu}\sum_1^{s_\mu}{}_{j'} \left|M \sum_1^{s_\nu}{}_i \left(\omega_{\nu i}, \exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j}\right)^* \times \left(\omega_{\nu i}, \exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j'}\right) - \frac{s_\nu}{S}\delta_{jj'}\right|^2 \ll \frac{1}{N}\frac{s_\nu^2}{S^2}. \tag{10″}$$

We notice that if, instead of (10′)(10″), one supposes the following much more restrictive condition, to be verified

$$M \sum_1^{s_\nu}{}_i \left(\omega_{\nu i}, \exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j}\right)^* \times \left(\omega_{\nu i}, \exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j'}\right) \cong \frac{s_\nu}{S}\delta_{jj'}, \tag{11}$$

then, as one can easily deduce from (9), condition (4) is satisfied for every initial condition and not only for the overwhelming majority of these.[5]

[5] Starting from an initial state vector of the following type:

$$\psi_0 = \sum_1^N{}_\mu [u_\mu(0)]^{\frac{1}{2}}\psi_{0\mu},$$

where $\psi_{0\mu}$ is normalized and belongs to V_μ and denoting now by $\mathfrak{B}$ an average, by letting each $\psi_{0\mu}$ vary independently within the cell V_μ whole keeping $u_\mu(0)$ constant. Relation (4) may be still satisfied if one substitutes (10″) with the following relation,

3. DISCUSSION OF THE RESULTS

To understand the meaning of the ergodicity conditions derived in the previous section, let us begin by discussing condition (11) which is the simplest formally.

For $j=j'$ the left-hand side of (11) becomes the time average of the norm of $\omega_{\mu j}$ time evolved and projected on to the cell V_ν. Such a condition requires, therefore, that this quantity be proportional to the dimensions of the cell V_ν whatever the values of μ and j; that is to say that no cell may be particularly preferred in the course of the time evolution of $\omega_{\mu j}$.

For $j\neq j'$, the left-hand side of (11) becomes the time average of the scalar product of $\omega_{\mu j}$ and $\omega_{\mu j'}$ time evolved and projected on to V_ν. Condition (11) then requires that there be no appreciable correlation between the directions of these two vectors.

Conceptually conditions (10′), (10″) are similar to (11); they contain, however, averages over the values of j and j' relative to a given cell V_μ; that is, they are therefore much less restrictive, as one can see immediately, if one realizes that reasonable values for s_μ are, for instance, of the order of $e^{10^{20}}$.

We emphasize that (10′), (10″) are the most general ergodicity conditions. Their analytical structure can be better understood by giving them another form. To this end let us consider the spectral decomposition of the Hamiltonian

$$H=\sum_1^S{}_\rho\, E_\rho P_\rho,$$

where P_ρ is the projection operator on the manifold of eigenstates belonging to the eigenvalue E_ρ; we have then

$$\exp\left(-\frac{i}{\hbar}Ht\right)=\sum_1^S{}_\rho \exp\left(-\frac{i}{\hbar}E_\rho t\right)P_\rho;$$

thus $(M\exp[-(i/\hbar)(E_\rho-E_\sigma)t]=\delta_{\rho\sigma})$, (10′), (10″) become

$$\left|\frac{1}{s_\mu}\sum_1^{s_\mu}{}_j\sum_1^S{}_\rho\sum_1^{s_\nu}{}_i|(\omega_{\nu i},P_\rho\omega_{\mu j})|^2-\frac{s_\nu}{S}\right|\ll\frac{1}{N^{\frac{1}{2}}}\frac{s_\nu}{S},\quad(12')$$

which is a little more general:

$$\frac{1}{s_\mu}\sum_1^{s_\mu}{}_j\frac{1}{s_{\mu'}}\sum_1^{s_{\mu'}}{}_{j'}\left|M\sum_1^{s_\nu}{}_i\left(\omega_{\nu i},\exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j}\right)^*\times\left(\omega_{\nu i},\exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu' j'}\right)-\frac{s_\nu}{S}\delta_{\mu\mu'}\delta_{jj'}\right|^2\ll\frac{1}{N}\frac{s_\nu^2}{S^2}.$$

However, these relations have only a formal interest in view of the fact that, from a physical point of view, no particular meaning may be attributed to state vectors of this type.

$$\frac{1}{s_\mu}\sum_1^{s_\mu}{}_j\frac{1}{s_\mu}\sum_1^{s_\mu}{}_{j'}\left|\sum_1^S{}_\rho\sum_1^{s_\nu}{}_i(\omega_{\nu i},P_\rho\omega_{\mu j})^*(\omega_{\nu i},P_\rho\omega_{\mu j'})-\frac{s_\nu}{S}\delta_{jj'}\right|^2\ll\frac{1}{N}\frac{s_\nu^2}{S^2}.\quad(12'')$$

If we assume that there are no degeneracies and denote by $U_{\rho;\nu i}$ the unitary matrix, which connects the energy eigenvectors with the basis $\omega_{\nu i}$, we obtain

$$M\sum_1^{s_\nu}\left(\omega_{\nu i},\exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j}\right)^*\times\left(\omega_{\nu i},\exp\left(-\frac{i}{\hbar}Ht\right)\omega_{\mu j'}\right)=\sum_1^S{}_\rho\, U_{\rho;\mu j}{}^*U_{\rho;\mu j'}\sum_1^{s_\nu}{}_i|U_{\rho;\nu i}|^2.$$

Condition (11) becomes then, under this assumption, equivalent to the ergodicity condition given by Fierz[6]

$$\sum_1^{s_\nu}{}_i|U_{\rho;\nu i}|^2\cong\frac{s_\nu}{S}.$$

From (12′) (12″) one can see that our ergodicity conditions are essentially conditions on the spectral family of the Hamiltonian of the system, they are then connected in a rather complicated way to the structure of the Hamiltonian itself, and it does not seem an easy task to show that they are actually satisfied in the case of systems physically interesting such as, for instance, a gas of weakly interacting particles.

This, no doubt, is their essential drawback.

However, one should not forget that such a situation is not different from that of classical statistical mechanics where no criterion has yet been found to single out metrically transitive systems. (Metrical transitivity, in fact, is the ergodicity condition generally assumed in classical statistical mechanics.)

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[6] M. Fierz, Helv. Phys. Acta 28, 705 (1955).

Proof of Carathéodory's Local Theorem and Its Global Application to Thermostatics

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It is pointed out that Carathéodory's proof of his theorem on pfaffian forms, which was used in his axiomatic development of thermostatics, is not complete and does not make clear whether this result is valid locally or globally. This theorem is replaced by a more precise statement of a local nature, for which a proof is given. By tracing through Carathéodory's use of the concept of thermal equilibrium with respect to simple systems, it is shown how the existence of a global entropy and absolute temperature may be deduced from this local result.

1. INTRODUCTION

IN 1909 Carathéodory proposed an axiomatic foundation of thermostatics.[1] In this work he stated a theorem on pfaffian forms, known subsequently as Carathéodory's theorem, but mathematicians have found his proof to be incomplete. Moreover, it is not made clear either in the original or subsequent treatments of Carathéodory's approach[2-5] whether this result is local or global. In Sec. 2 of this article, we shall restate the theorem more precisely as a local theorem and shall give a proof of our statement in Sec. 3. In the final section, we shall discuss how this local theorem finds a global application in thermostatics through the use of Carathéodory's assumptions on thermal equilibrium.

2. CARATHÉODORY'S THEOREM

We quote Carathéodory's theorem[1]:
"Let a pfaffian equation

$$dx_0+X_1dx_1+\cdots+X_ndx_n=0 \tag{2.1}$$

be given, where the X_i are finite, continuous, differentiable functions of the x_i, and it is known that in every neighborhood of an arbitrary point P in the space of the x_i, there are points which cannot be reached along curves which satisfy this equation, then there must be a multiplier of the expression (2.1) which makes it an exact differential."

In the course of his argument, Carathéodory appears to establish that on the line $x_0=t$, $x_k=a_k$, $k=1, \cdots, n$, there is exactly one point which can be reached from a given point $a_0, a_1, \cdots, a_n$ along a curve satisfying (2.1). This would indeed show that the coordinates of the points which can be thus reached from P satisfy an equation of the form

$$F(x_0,x_1,\cdots,x_n)=0,$$

but it is not shown that F is a smooth function, which would be required for the remaining part of his proof. Without doubt, this single gap could be bridged with some further work on his proof, but additional difficulties would remain, and the process of removing them could become tedious. Hence we have chosen to replace his argument with one of a different nature. Besides, neither Carathéodory's statement nor his proof clarifies the question of whether his result should be interpreted locally or globally. Thus we shall demonstrate, instead of the theorem quoted in the foregoing, a more precise statement which we call *Carathéodory's Local Theorem: Let*

$$DP=\sum_{i=1}^{n} P_idx_i \tag{2.2}$$

be a given pfaffian form in a region G of the space whose points have coordinates $x_1, \cdots, x_n$. *Suppose that the* P_i *are infinitely often differentiable functions of the* x_i *and that* $\sum_{i=1}^{n} P_iP_i>0$ *in G. Suppose further that in every neighborhood R of an arbitrary point* $\mathbf{a}\in G$ *there exists another point in R which cannot be joined to* **a** *by a piecewise smooth curve satisfying* $\sum_{i=1}^{n}P_idx_i=0$, *and lying entirely in R. Then in some neighborhood of* **a** *there are functions* $\lambda(x_i)$ *and* $\varphi(x_i)$ *such that*

$$DP=\lambda d\varphi.$$

The proof of this theorem is the subject of the next section.

3. PROOF OF CARATHÉODORY'S LOCAL THEOREM

We quote a theorem on pfaffian forms:
Every pfaffian form

$$\omega=g_1df_1+\cdots+g_mdf_m,$$

in which the symbols which occur, f_i, g_i, *are infinitely often differentiable functions of n independent variables, say* $u_1, \cdots, u_n$, *can be put into one or the other of the following forms (in some neighborhood of each point)*[6]

$$\omega=dz_1+y_2dz_2+\cdots+y_pdz_p, \tag{3.1}$$

$$\omega=y_1dz_1+\cdots+y_pdz_p. \tag{3.2}$$

[1] C. Carathéodory, Math. Ann. 67, 355 (1909).
[2] M. Born, Physik. Z. 22, 218–225, 249–254, and 282–286 (1921).
[3] C. Carathéodory, *Über die Bestimmung der Energie und der absoluten Temperatur mit Hilfe von reversiblen Prozessen* (S. B. preuss Akad., 1925), pp. 39–47.
[4] S. Chandrasekhar, *An Introduction to the Study of Stellar Structure* (University of Chicago Press, Chicago, Illinois, 1939).
[5] A. H. Wilson, *Thermodynamics and Statistical Mechanics* (Cambridge University Press, New York, 1957).
[6] C. Carathéodory, *Variationsrechnung und Partielle Differentialgleichungen Erster Ordnung* (B. G. Teubner, Leipzig, Germany, 1956), Vol. 1.

In each of these expressions, the symbols which occur y_i, z_i are mutually independent (infinitely often differentiable functions of $u_1, \cdots, u_n$).

We shall see that our theorem follows almost immediately from this one.

Consider a point $\mathbf{a} \epsilon G$. Then in some neighborhood, H of $\mathbf{a}$ we may write either

$$DP = \sum_{i=1}^{r+1} \lambda_i d\varphi_i, \quad \text{(case I)},$$

or

$$DP = d\varphi_1 + \sum_{i=2}^{r+1} \lambda_i d\varphi_i, \quad \text{(case II)},$$

in general, where, in accordance with the theorem quoted in the foregoing, all of the λ_k and φ_k occurring are independent functions of $x_1, \cdots, x_n$. In case I, we must have at least one of the $\lambda_i > 0$ at $\mathbf{a}$, since

$$\sum_{i=1}^{n} P_i P_i > 0.$$

We may assume in this case, without loss of generality, that $\lambda_1 > 0$ at $\mathbf{a}$, and that H is so chosen that $\lambda_1 > \epsilon > 0$ in H, where ϵ is some positive number. Then define

$$DQ = DP \quad \text{(case I)},$$

or

$$DQ = DP/\lambda_1 \quad \text{(case II)}$$

in H, so that DQ has the form

$$DQ = d\bar{\alpha} + \sum_{j=1}^{r} \bar{p}_j d\bar{q}_j, \tag{3.3}$$

in general, where $\bar{\alpha}, \bar{p}_j, \bar{q}_j, j = 1, \cdots, r$, are independent functions of the x_i and DQ satisfies the hypotheses of Carathéodory's local theorem in H. We shall show that actually $DQ = d\bar{\alpha}$, and that the $\bar{p}_j$ and $\bar{q}_j$ cannot occur.

Suppose that there is at least one $\bar{p}_j$ and $\bar{q}_j$ occurring in (3.3). Then choose $v_{2r+2}, \cdots, v_n$ so that $\bar{\alpha}, \bar{p}_j, \bar{q}_j, \bar{v}_k$, $j = 1, \cdots, r$, $k = 2r+2, \cdots, n$, form a set of independent functions in some neighborhood $\bar{H}$ of $\mathbf{a}$ contained in H, and take them to be coordinates there. Let these coordinates of $\mathbf{a}$ be given by ${}_a\bar{\alpha}, {}_a\bar{p}_j, {}_a\bar{q}_j, {}_a\bar{v}_k$. Make the further coordinate transformation

$$\alpha = \bar{\alpha} - {}_a\alpha + \sum_{j=1}^{r} {}_a\bar{p}_j(\bar{q}_j - {}_a\bar{q}_j),$$

$$p_i = \bar{p}_i - {}_a\bar{p}_i, \quad q_i = \bar{q}_i - {}_a\bar{q}_i, \quad v_k = \bar{v}_k - {}_a\bar{v}_k,$$

$$i = 1, \cdots, r, \quad k = 2r+2, \cdots, n.$$

Then the coordinates of $\mathbf{a}$ all become zero; also

$$DQ = d\alpha + \sum_{j=1}^{r} p_i dq_i.$$

Consider now a neighborhood N of $\mathbf{a}$, contained in $\bar{H}$, of the form

$$-l^2 < \alpha < l^2, \quad -2l < p_i < 2l, \quad -l < q_i < l, \quad -l < v_k < l,$$

where l is some positive number. Given any point $\mathbf{b} \epsilon N$, with coordinates ${}_b\alpha, {}_bp_i, {}_bq_i, {}_bv_k$, we shall now construct a curve $C \epsilon N$, satisfying the pfaffian equation $DQ = 0$, and joining $\mathbf{a}$ to $\mathbf{b}$. Let C consist of the five smooth parts, $C_1, \cdots, C_5$ defined as follows, where $i = 1, \cdots, r$, $k = 2r+2, \cdots, n$

C_1: $\alpha = 0$, $p_1 = -tl$, $p_2 = \cdots = p_r = 0$, $q_i = 0$, $v_k = 0$; $0 \leq t \leq 1$.

C_2: $\alpha = {}_b\alpha(t-1)$, $p_1 = -l$, $p_2 = \cdots = p_r = 0$, $q_1 = l^{-1}{}_b\alpha(t-1)$, $q_2 = \cdots = q_r = 0$, $v_k = 0$; $1 \leq t \leq 2$.

C_3: $\alpha = {}_b\alpha$, $p_1 = l(t-3)$, $p_2 = \cdots = p_r = 0$, $q_1 = l^{-1}{}_b\alpha$, $q_2 = \cdots = q_r = 0$, $v_k = 0$; $2 \leq t \leq 3$.

C_4: $\alpha = {}_b\alpha$, $p_i = 0$, $q_1 = l^{-1}{}_b\alpha(4-t) + {}_bq_1(t-3)$, $q_l = {}_bq_l(t-3)$, $v_k = 0$, $3 \leq t \leq 4$.

C_5: $\alpha = {}_b\alpha$, $p_i = {}_bp_i(t-4)$, $q_i = {}_bq_i$, $v_k = {}_bv_k(t-4)$, $4 \leq t \leq 5$.

But the existence of the curve C violates our hypotheses. Thus the only alternative is that (3.3) read $dQ = d\bar{\alpha}$, or either $DP = \lambda_1 d\varphi_1$ (case I) or $DP = d\varphi_1$ (case II). On defining $\lambda = \lambda_1$ in case I, $\lambda = 1$ in case II, and $\varphi = \varphi_1$ in both cases, we get $DP = \lambda d\varphi$ in H, and hence the theorem is proven.

4. GLOBAL APPLICATION OF CARATHÉODORY'S THEOREM IN THERMOSTATICS

This, our concluding section, is devoted to a remark on how the local Carathéodory theorem is applied globally in the space of states of a system through the use of the concept of thermal equilibrium. The development is essentially that of Carathéodory,[1] but the remarks on local and global interpretations are ours.

Carathéodory considers simple systems which, as far as we are concerned, are pfaffian forms of the type

$$dE + \sum_{i=1}^{n} X_i dV_i, \tag{4.1}$$

where n may take values 1, 2, $\cdots$. The X_i are functions of $E, V_1, \cdots, V_n$. These forms constitute a class with the following properties of interest to us:

(a) The hypotheses, and, hence, conclusions, of Carathéodory's local theorem, hold for all forms in this class.

(b) There exists a quantity θ, called the empirical temperature, expressible as a function of $E, V_1, \cdots, V_n$, i.e., $\theta = f(E, V_1, \cdots, V_n)$, such that the rank of the matrix

$$\begin{pmatrix} \partial f/\partial E & \partial f/\partial V_1 & \cdots & \partial f/\partial V_n \\ E & V_1 & \cdots & V_n \end{pmatrix} \tag{4.2}$$

is two.

(c) From any two forms in the class

$$dE'+\sum_{i=1}^{N'} X_i'dV_i', \tag{4.3}$$

$$dE''+\sum_{j=1}^{N''} X_j''dV_j'', \tag{4.4}$$

we may construct a third form

$$d\bar{E}+\sum_{i=1}^{N'} X_i'dV_i'+\sum_{j=1}^{N''} X_j''dV_j'', \tag{4.5}$$

where $\bar{E}=E'+E''$, and the quantities

$$E',\ E'',\ V_i',\ V_j'',\quad i=1,\cdots,N',\quad j=1,\cdots,N''$$

are related by

$$'\theta(E',V_1',\cdots,V_{N'}')={}''\theta(E'',V_1'',\cdots,V_{N''}''), \tag{4.6}$$

where the left- and right-hand sides of (4.6) are functions which give the empirical temperatures for (4.3) and (4.4), respectively. The empirical temperature of (4.5) must then also be equal to either side of (4.6). (The physical idea involved here is, of course, the formation of a system by putting two given systems into thermal contact with each other.)

E is called the internal energy, $V_1,\ \cdots,\ V_n$ the deformation coordinates, and $X_1,\ \cdots,\ X_n$ are called forces. A value of $E,\ V_1,\ \cdots,\ V_n$ is called a state. The condition on the rank of the matrix (4.2) insures that there is a path through each state along which (4.1) vanishes, but θ is not constant and vice versa. [Physically this means that an isothermal process through a given state need not coincide with a quasistatic adiabatic process, which is a curve along which (4.1) vanishes.] Also the rank condition on (4.2) ensures that E' and E'' are determined by $V_1',\ \cdots,\ V_{N'}',\ \theta$ and $V_1'',\ \cdots,\ V_{N''}'',\ \theta$, respectively, and, hence, because of (c), by $\bar{E},\ V_1',\ \cdots,\ V_{N''}''$.

From these considerations, (a), and Carathéodory's local theorem, we see that for some neighborhood of a given state of the system (4.5) there exist state functions $\tilde{\lambda}$ and $\tilde{\sigma}$ such that (4.5) becomes $\tilde{\lambda}d\tilde{\sigma}$. But this given state of (4.5) determines states of (4.3) and (4.4), for some neighborhoods of which (4.3) and (4.4) become $\lambda'd\sigma'$ and $\lambda''d\sigma''$, respectively. Thus for some neighborhood of a given state of (4.5), we have

$$\tilde{\lambda}d\tilde{\sigma}=\lambda'd\sigma'+\lambda''d\sigma''. \tag{4.7}$$

Now because of the condition on the rank of (4.2), we may locally transform the independent variables of (4.3) and (4.4) to say, $\sigma',\ \theta,\ y_3',\ \cdots,\ y_N'$ and $\sigma'',\ \theta,\ y_3'',\ \cdots,\ y_N''$, all of which are independent. Thus (4.7) yields

$$\partial\sigma/\partial\sigma'=\lambda'/\lambda,\quad \partial\sigma/\partial\sigma''=\lambda''/\lambda,\quad \partial\sigma/\partial\theta=0, \tag{4.8}$$

from which we get

$$\partial(\lambda'/\lambda)/\partial\theta=\partial(\lambda''/\lambda)/\partial\theta=0,$$

which implies

$$\partial\ \ln\lambda/\partial\theta=\partial\ \ln\lambda'/\partial\theta=\partial\ \ln\lambda''/\partial\theta. \tag{4.9}$$

But since λ' does not depend on $\sigma'',\ y_3'',\ \cdots,\ y_{N''}''$ and λ'' does not depend on $\sigma',\ y_3',\ \cdots,\ y_N'$, we get from (4.9)

$$\partial\ \ln\lambda'/\partial\theta=F(\theta)=\partial\ \ln\lambda'/\partial\theta,$$

which yields relations of the form

$$\lambda'=L(\theta)\ 'G(\sigma',y_3,\cdots,y_{N'}'), \tag{4.10}$$

$$\lambda''=L(\theta)\ ''G(\sigma'',y_3'',\cdots,y_{N''}''). \tag{4.11}$$

But from (4.7) we get also

$$\partial\sigma/\partial y_3'=0,$$

which, when combined with $(4.8)_1$ and $(4.8)_2$, yields

$$\partial\ \ln\lambda/\partial y_3'=\partial\ \ln\lambda'/\partial y_3'=\partial\lambda''/\partial y_3'=0,$$

the last equality following since λ'' does not depend on y_3''. Hence (4.10) becomes

$$\lambda'=L(\theta)G(\sigma',y_4',\cdots,y_{N'}').$$

By continuing this process we get

$$\lambda'=L(\theta)\ 'G(\sigma'),\quad \lambda''=L(\theta)\ ''G(\sigma''),$$

and hence

$$\lambda'd\sigma'=L(\theta)d\int {}'G(\sigma')d\sigma',$$

$$\lambda''d\sigma''=L(\theta)d\int {}''G(\sigma'')d\sigma''.$$

Thus $[L(\theta)]^{-1}$ is a possible integrating factor for both (4.3) and (4.4). Since the ratio of two integrating factors of (4.5) must be a function of σ', $L(\theta)$ is determined to within a multiplicative constant.

Now since $L(\theta)$ is known as a point function, once we specify the multiplicative constant, then we see that $L(\theta)$ is a global integrating factor, not only for the forms (4.3) and (4.4), but for all simple systems. The local considerations have gone out in the wash. When the constant is properly fixed, $L(\theta)$ is called the absolute temperature, and $[L(\theta)]^{-1}$ multiplied by (4.1) yields an exact differential expression for the entropy, which is *globally* determined.

Numerical Integration of the Transport Equation with No Angular Truncation*

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For any given azimuth-independent scattering law, it is shown that the neutron transport equation with external source is rigorously equivalent to a coupled system of Fredholm integral equations. These are derived both for vacuum and periodic boundary conditions. A numerical integration scheme is given for solving these integral equations with no angular truncation error, thereby permitting the solution of the Boltzmann equation numerically, with no error but that in the spatial integration. All cross sections are permitted to be arbitrarily given functions of position, if desired.

I. INTRODUCTION

IN recent years, numerous methods have been proposed for the numerical integration of the neutron transport equation. Among these, the most successful have probably been the S_n method of Carlson,[1] the D_n (discrete ordinate) method of Wick-Chandrasekhar,[2–4] and the P_n (spherical harmonics) method.[5] In each of these, one first approximates the many-velocity Boltzmann equation by a sequence of coupled one-velocity equations, thereby reducing the problem to that of integrating the one-velocity equation with given source. The next step is to approximate the angular flux $\psi(x,\omega)$ in some manner, whose accuracy is indicated by the subscript n.

Thus in the S_n method, one assumes that the flux is, for each x, sectionally linear in ω, with n sections. In the D_n method, $\psi(x,\omega)$ is approximated by an interpolating polynomial over the full range $-1\leqq\omega\leqq 1$ of degree n. Finally, the P_n is equivalent to the D_n method from the point of view of the angle approximation.[6] The effect of these approximations is, in each case, to permit the angle integration appearing in the transport equation [(1), *infra*] to be done, and thereby to reduce that equation to a system of coupled linear ordinary differential equations in the space variable x, only, which are then integrated numerically.

The method presented in this paper also deals with the one-velocity transport equation, and therefore, as regards the energy approximation, it is heir to all the ills which beset the procedures mentioned in the foregoing.

The only angle approximation we make in the one-velocity equation, however, is that the spherical harmonics expansion of the scattering kernel is permitted to contain only finitely many harmonics. Subject only to this approximation, we will integrate numerically a system of integral equations which is rigorously equivalent to the transport equation. To put it otherwise, we will obtain the exact solution of an approximate problem in which the true scattering materials are replaced by fictitious ones whose scattering laws are not "too anisotropic."

This idea has already been used by several authors for purposes other than numerically integrating the transport equation. Thus it appears already in Bethe, Tonks, and Hurwicz,[7] and was used by Hurwitz and Zweifel.[8,9] The latter authors assumed a sinusoidal source in the many velocity equation, truncated the scattering kernel as we do below, and reduced the problem, for an infinite medium, to a system of integral equations in the lethargy. Our procedure is therefore more special, in that energy variation is not allowed, but more general in that finite, stratified media are considered along with arbitrary angle and position variation of the source.

The numerical method chosen for solving the integral equations below is, in essence, the well-known method of multiple collisions, together with a numerical integration scheme explicitly devised for the purpose of dealing with singularities in the kernels of the equations. The multiple collision method, while always convergent for subcritical systems, may be only slowly convergent for nearly critical assemblies. As a result of experience gained with this method in a slightly simpler context (see footnote reference 4, p. 308), it seems fair to assert that in most cases arising in practice, even in deep penetration problems, convergence will be sufficiently rapid to permit the method to be used. This favorable state of affairs apparently results from the fact that each one-velocity problem being solved, usually represents *in itself* a strongly subcritical system even though, considered as a many-velocity entity, the reactor may be nearly critical.

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[1] B. Carlson, "A solution of the transport equation by S_n approximations," LA 1891 (1955).
[2] G. C. Wick, Z. Physik, **121**, 702 (1943).
[3] S. Chandrasekhar, *Radiative Transfer* (Oxford University Press, New York, 1950).
[4] H. S. Wilf, Nuclear Sci. and Eng. **5**, 5 (1959).
[5] B. Davison, *Neutron Transport Theory* (Oxford University Press, New York, 1957).
[6] G. Goertzel, Nuclear Sci. and Eng. 4, 581 (1958).
[7] H. A. Bethe, L. Tonks, and H. Hurwitz, Jr., Phys. Rev. **80**, 11 (1950).
[8] H. Hurwitz and P. Zweifel, J. Appl. Phys. **25**, 1241 (1954).
[9] H. Hurwitz and P. Zweifel, J. Appl. Phys. **26**, 923 (1955).

II. THE PROBLEM

The transport equation is

$$\omega\frac{\partial\psi(x,\omega)}{\partial x}+\mu(x)\psi(x,\omega)=\int_{-1}^{1}K(x,\omega,\omega')\psi(x,\omega')d\omega'+s(x,\omega), \quad (1)$$

where the symbols are ω cosine of angle with positive x axis; x x coordinate; $\psi(x,\omega)$ flux density of neutrons at position x, traveling in direction ω; $\mu(x)$ total cross section; $K(x,\omega,\omega')$ scattering kernel; and $s(x,\omega)$ external source density.

If the scattering is azimuth-independent we can always write

$$K(x,\omega,\omega')=\sum_{l=0}^{\infty}b_l(x)P_l(\omega)P_l(\omega'). \quad (2)$$

We assume that data concerning the $b_l(x)$ are unknown, unreliable, or rigorously absent beyond $l=L$, so that

$$K(x,\omega,\omega')=\sum_{l=0}^{L}b_l(x)P_l(\omega)P_l(\omega'). \quad (3)$$

It should be noted, at this point, that (3) is no assumption about the angular flux, and that conventional methods, say the P_n method, do not give exact solutions for any finite n, even if $L=0$ (isotropic scattering).

For boundary conditions we adopt either of the sets

$$\left.\begin{array}{ll}\text{(a)}\ \psi(x,\omega)=0 & x=0;\ \omega>0\\ \text{(b)}\ \psi(x,\omega)=0 & x=A;\ \omega<0\end{array}\right\}\text{vacuum.} \quad (4)$$

$$\psi(0,\omega)=\psi(A,\omega)\quad\text{cell} \quad (5)$$

III. SUMMARY OF ANALYSIS

In the following sections we shall show that Eqs. (1), (3), and (4) are rigorously equivalent to

$$f_s(x)=\sum_{l=0}^{L}\int_0^A b_l(x')Q_{ls}(|\tau(x,x')|)f_l(x')dx'+\rho_s(x), \quad (s=0,1,\cdots) \quad (6)$$

where

$$Q_{ls}(|\tau(x,x')|)=\begin{cases}K_{ls}(|\tau(x,x')|) & l+s\ \text{even}\\ sgn(x-x')K_{ls}(|\tau(x,x')|) & l+s\ \text{odd}\end{cases} \quad (7)$$

$$K_{ls}(t)=\int_0^1 P_l(\omega)\left[\frac{1}{\omega}-e^{-t/\omega}\right]P_s(\omega)d\omega \quad (8)$$

$$\tau(x,x')=\int_{x'}^{x}\mu(x'')dx'' \quad (9)$$

$$f_l(x)=\int_{-1}^{1}P_l(\omega)\psi(x,\omega)d\omega \quad (10)$$

$$\rho_s(x)=\sum_{l=0}^{\infty}\int_0^A Q_{ls}(|\tau(x,x')|)s_l(x')dx' \quad (11)$$

$$s(x,\omega)=\sum_{l=0}^{\infty}s_l(x)P_l(\omega). \quad (12)$$

The salient feature of the system of integral equations (6) is that they are coupled only for $s=0, 1, \cdots, L$, while for $s>L$, they simply give $f_s(x)$ as a quadrature of $f_0(x), \cdots, f_L(x)$. Because of this, one need only solve the first $L+1$ of these equations in order to know the total flux $f_0(x)$ and current $f_1(x)$ exactly. A numerical procedure for solving the system is given in Sec. VIII.

It is also remarkable that for the cell boundary conditions (5) Eqs. (6), (7), (9), (10), (11), and (12) are unchanged, with (8) changing to

$$K_{ls}^*(t)=\int_0^1 P_l(\omega)\left[\frac{1}{\omega}\frac{1}{1-e^{-\tau_0/\omega}}e^{-t/\omega}\right]P_s(\omega)d\omega, \quad (8)'$$

where

$$\tau_0=\tau(A,0)=\int_0^A\mu(x)dx \quad (13)$$

is the thickness of the cell, in mean free paths. This simple change means that a computer code can easily have a built-in option for the boundary conditions desired.

IV. DERIVATION FOR VACUUM BOUNDARY CONDITIONS

By substituting (3) and (10) into (1),

$$\omega\frac{\partial\psi}{\partial x}+\mu\psi=\sum_{l=0}^{L}b_l(x)P_l(\omega)f_l(x)+s(x,\omega)=\omega\exp\left\{-\int_0^x\frac{\mu(x')}{\omega}dx'\right\}\times\frac{\partial}{\partial x}\left\{\psi(x,\omega)\exp\left[\int_0^x\frac{\mu(x')}{\omega}dx'\right]\right\}. \quad (14)$$

Thus

$$\frac{\partial}{\partial x}\left\{\psi(x,\omega)\exp\left[\int_0^x\frac{\mu(x')}{\omega}dx'\right]\right\}=\frac{1}{\omega}\exp\left[\int_0^x\frac{\mu(x')}{\omega}dx'\right]\times\left\{\sum_{l=0}^{L}b_l(x)P_l(\omega)f_l(x)+s(x,\omega)\right\}. \quad (15)$$

Suppose $\omega>0$. On integrating (15) from 0 to x, and using (4) (a), and (9),

$$\psi(x,\omega)=\frac{1}{\omega}\int_0^x \exp\left[-\frac{\tau(x,x')}{\omega}\right] \times\left\{\sum_{l=0}^{L} b_l(x')P_l(\omega)f_l(x')+s(x',\omega)\right\}dx' \quad (\omega>0). \quad (16)$$

If $\omega<0$, integrate (15) from x to A, use (4) (b) and (9), getting

$$\psi(x,\omega)=-\frac{1}{\omega}\int_x^A \exp\left[-\frac{\tau(x,x')}{\omega}\right] \times\left\{\sum_{l=0}^{L} b_l(x')P_l(\omega)f_l(x')+s(x',\omega)\right\}dx' \quad (\omega<0). \quad (17)$$

By analogy with (10), define

$$f_l^+(x)=\int_0^1 P_l(\omega)\psi(x,\omega)d\omega \quad (18)$$

$$f_l^-(x)=\int_{-1}^0 P_l(\omega)\psi(x,\omega)d\omega. \quad (19)$$

Upon multiplying (16) by $P_s(\omega)d\omega$ and integrating over $[0,1]$,

$$f_s^+(x)=\int_0^x \sum_{l=0}^{L} b_l(x')f_l(x') \times\left[\int_0^1 \frac{1}{\omega}\exp\left\{-\frac{\tau(x,x')}{\omega}\right\}P_l(\omega)P_s(\omega)\right]d\omega dx' +\int_0^x\int_0^1 \frac{1}{\omega}\exp\left\{-\frac{\tau(x,x')}{\omega}\right\}P_s(\omega)s(x',\omega)d\omega dx'. \quad (20)$$

By multiplying (17) by $P_s(\omega)d\omega$ and integrating over $[-1,0]$,

$$f_s^-(x)=\int_x^A \sum_{l=0}^{L} b_l(x')f_l(x') \times\left[-\int_{-1}^0 \frac{1}{\omega}\exp\left\{-\frac{\tau(x,x')}{\omega}\right\}P_l(\omega)P_s(\omega)d\omega\right]dx' +\int_x^A\int_{-1}^0 -\frac{1}{\omega}\exp\left\{-\frac{\tau(x,x')}{\omega}\right\}P_s(\omega)s(x',\omega)d\omega dx'. \quad (21)$$

In (21), $x'>x$, thus $\tau(x,x')<0$ and $-\tau(x,x')=|\tau(x,x')|$. Hence in (21) we may write

$$-\int_{-1}^0 \frac{1}{\omega}\exp\left\{-\frac{\tau(x,x')}{\omega}\right\}P_l(\omega)P_s(\omega)d\omega =-\int_1^0 -\frac{1}{\omega}\exp\left\{-\frac{|\tau(x,x')|}{\omega}\right\}P_l(-\omega)P_s(-\omega)d(-\omega) =(-1)^{l+s}\int_0^1 \frac{1}{\omega}\exp\left\{-\frac{|\tau(x,x')|}{\omega}\right\}P_l(\omega)P_s(\omega)d\omega. \quad (22)$$

Let us define, for $t>0$, $K_{ls}(t)$ by (8). By using (12) we obtain (20) and (21) in the form

$$f_s^+(x)=\int_0^x \sum_{l=0}^{L} b_l(x')f_l(x')K_{ls}(|\tau(x,x')|)dx' +\int_0^x \sum_{l=0}^{\infty} s_l(x')K_{ls}(|\tau(x,x')|)dx' \quad (23)$$

$$f_s^-(x)=\int_x^A \sum_{l=0}^{L} b_l(x')f_l(x')(-1)^{l+s}K_{ls}(|\tau(x,x')|)dx' +\int_x^A \sum_{l=0}^{\infty} s_l(x')(-1)^{l+s}K_{ls}(|\tau(x,x')|)dx,' \quad (24)$$

whence the final result (6) follows by addition of (23) and (24).

V. KERNELS $K_{ls}(t)$

Suppose numbers α_{ln} are defined by

$$P_l(\omega)=\sum_{n=0}^{l}\alpha_{ln}\omega^n; \quad \alpha_{ln}=0 \quad (n>l). \quad (25)$$

Then, if $l\geqq s$,

$$P_l(\omega)P_s(\omega)=\sum_{n=0}^{l}\alpha_{ln}\omega^n\sum_{m=0}^{l}\alpha_{sm}\omega^m =\sum_{n=0}^{2l}\beta_{nls}\omega^n,$$

where

$$\beta_{nls}=\sum_{\alpha=0}^{n}\alpha_{lj}\alpha_{s,n-j}.$$

Hence

$$K_{ls}(t)=\sum_{n=0}^{2l}\beta_{nls}\int_0^1 \omega^{n-1}e^{-t/\omega}d\omega=\sum_{n=0}^{2l}\beta_{nls}\int_1^\infty \frac{e^{-ty}}{y^{n+1}}dy,$$

or

$$K_{ls}(t)=\sum_{n=0}^{2l}\beta_{nls}E_{n+1}(t)=K_{sl}(t). \quad (26)$$

Thus each $K_{ls}(t)$ is a linear combination of E_n functions. The first few are

$$\left.\begin{aligned} K_{00}&=E_1(t)\\ K_{10}&=K_{01}=E_2(t)\\ K_{11}&=E_3(t)\\ K_{02}&=K_{20}=\tfrac{3}{2}E_3(t)-\tfrac{1}{2}E_1(t)\\ K_{12}&=K_{21}=\tfrac{3}{2}E_4(t)-\tfrac{1}{2}E_2(t)\\ K_{22}&=(9/4)E_5(t)-\tfrac{3}{2}E_3(t)+\tfrac{1}{4}E_1(t)\end{aligned}\right\}. \tag{27}$$

From the recurrence formula

$$(r+1)P_{r+1}(\omega)+rP_{r-1}(\omega)=(2r+1)\omega P_r(\omega),$$

we find

$$(l+1)K_{l+1,s}+lK_{l-1,s}=\int_0^1 (2l+1)\omega P_l(\omega)\frac{1}{\omega}e^{-t/\omega}P_s(\omega)d\omega$$

$$=(2l+1)\int_0^1 P_l(\omega)\frac{1}{\omega}e^{-t/\omega}\omega P_s(\omega)d\omega,$$

from which

$$\frac{l+1}{2l+1}K_{l+1,s}+\frac{l}{2l+1}K_{l-1,s}$$

$$=\frac{s+1}{2s+1}K_{l,s+1}+\frac{s}{2s+1}K_{l,s-1}. \tag{28}$$

VI. DERIVATION FOR CELL BOUNDARY CONDITIONS

With the boundary conditions (5) were turn again to (15), and for $\omega>0$ we integrate from 0 to x, getting

$$\psi(x,\omega)\exp\left[\int_0^x\frac{\mu(x')}{\omega}dx'\right]-\psi(0,\omega)$$

$$=\frac{1}{\omega}\int_0^x\exp\left[\int_0^{x'}\frac{\mu(x'')}{\omega}dx''\right]$$

$$\times\left\{\sum_{l=0}^{L}b_l(x')P_l(\omega)f_l(x')+s(x',\omega)\right\}dx'. \tag{29}$$

For $\omega<0$ we integrate from x to A, and get

$$\psi(A,\omega)\exp\left[\int_0^A\frac{\mu(x')dx'}{\omega}\right]-\psi(x,\omega)\exp\left[\int_0^x\frac{\mu(x')}{\omega}dx'\right]$$

$$=\frac{1}{\omega}\int_x^A\exp\left[\int_0^{x'}\frac{\mu(x'')}{\omega}dx''\right]$$

$$\times\left\{\sum_{l=0}^{L}b_l(x')P_l(\omega)f_l(x')+s(x',\omega)\right\}dx'. \tag{30}$$

Now in (29), set $x=A$, and solve for $\psi(0,\omega)$, using (5),

$$\psi(0,\omega)=\psi(A,\omega)$$

$$=\omega^{-1}\{e^{\tau_0/\omega}-1\}^{-1}\int_0^A\exp\left[\int_0^{x'}\frac{\mu(x'')}{\omega}dx''\right]$$

$$\times\left\{\sum_{l=0}^{L}b_l(x')P_l(\omega)f_l(x')+s(x',\omega)\right\}dx'. \tag{31}$$

On putting (31) into (29), (30)

$$\psi(x,\omega)\exp\left\{\int_0^x\frac{\mu(x')dx'}{\omega}\right\}$$

$$-\omega^{-1}\{e^{\tau_0/\omega}-1\}^{-1}\int_0^A\exp\left[\int_0^{x'}\frac{\mu(x'')dx''}{\omega}\right.$$

$$\times\left\{\sum_{l=0}^{L}b_l(x')P_l(\omega)f_l(x')+s(x',\omega)\right\}dx'$$

$$=\frac{1}{\omega}\int_0^x\exp\left\{\int_0^{x'}\frac{\mu(x'')dx''}{\omega}\right\}$$

$$\times\left\{\sum_{l=0}^{L}b_l(x')P_l(\omega)f_l(x')+s(x',\omega)\right\}dx' \tag{32}$$

and

$$e^{\tau_0/\omega}\left[\omega^{-1}\{e^{\tau_0/\omega}-1\}^{-1}\int_0^A\exp\left(\int_0^{x'}\frac{\mu(x'')dx''}{\omega}\right)\right.$$

$$\times\left\{\sum_{l=0}^{L}b_l(x')P_l(\omega)f_l(x')+s(x',\omega)\right\}dx'\Bigg]$$

$$-\psi(x,\omega)\exp\left\{\int_0^x\frac{\mu(x')dx'}{\omega}\right\}$$

$$=\frac{1}{\omega}\int_x^A\exp\left\{\int_0^{x'}\frac{\mu(x'')dx''}{\omega}\right\}$$

$$\times\left\{\sum_{l=0}^{L}b_l(x')f_l(x')P_l(\omega)+s(x',\omega)\right\}dx'. \tag{33}$$

The result now follows from solving Eqs. (32) and (33) for $\psi(x,\omega)$, and treating the resulting equations exactly as Eqs. (16) and (17) were dealt with previously. The final result is given by Eq. (8)′.

VII. KERNELS $K_{ls}^*(t)$

The additional factor $[1-\exp-(\tau_0/\omega)]^{-1}$ in the definition of $K_{ls}^*(t)$ is readily understood physically as the sum of a geometric series, each term of which represents the interaction between the nth cell and the given cell.

Thus we write

$$K_{ls}^*(t)=\int_0^1 P_l(\omega)\left[\frac{1}{\omega}\frac{1}{1-e^{-\tau_0/\omega}}e^{-t/\omega}\right]P_s(\omega)d\omega$$
$$=\sum_{r=0}^{\infty}\int_0^1 P_l(\omega)\frac{1}{\omega}\exp\left\{-\frac{t+r\tau_0}{\omega}\right\}P_s(\omega)d\omega$$
$$=\sum_{r=0}^{\infty}K_{ls}(t+r\tau_0). \tag{34}$$

To see how rapidly this series converges, remembering that K_{ls} is a linear combination of E_n functions, consider

$$H_n(t)=\sum_{r=0}^{\infty}E_n(t+r\tau_0)\quad(n\geqq 1). \tag{35}$$

Now when its argument is large,

$$E_n(t+r\tau_0)\sim\frac{e^{-(t+r\tau_0)}}{t+r\tau_0+n},$$

so that (34) converges, ultimately, faster than a geometric series. For thick cells (weak interaction) a few terms suffice, while for thin cells many terms may be needed for sufficient accuracy.

VIII. NUMERICAL PROCEDURE

The numerical method adopted for the solution of the Fredholm system (6) is the development of the Neumann series, otherwise known as the method of multiple collisions. This choice was motivated primarily by considerations of programming simplicity.

On taking any initial guess

$$f_s^{(0)}(x)\quad(s=0,1,\cdots,L), \tag{35}$$

which may be zero if no better information is available, we calculate recursively

$$f_s^{(r+1)}(x)=\sum_{l=0}^{L}\int_0^A b_l(x')Q_{ls}(|\tau(x,x')|)f_l^{(r)}(x')dx' + \rho_s(x)\quad(s=0,1,\cdots,L). \tag{36}$$

The well-known theory of Fredholm equations assures us that

$$\lim_{r\to\infty}f_s^{(r)}(x)=f_s(x)\quad(s=0,1,\cdots,L), \tag{37}$$

where $f_s(x)$ satisfies (6), convergence being guaranteed whenever the reactor (considered as a one-velocity configuration) is subcritical. The iterative process (35)–(36) may therefore be continued until successive iterates agree sufficiently well, and the entire procedure has now been reduced to the question of the means of carrying out the numerical quadrature indicated in (36).

Naturally, this could be done by any standard method, but special steps would need to be taken, for the point $x'=x$, since at that point, reference to (27) shows that many of the kernels are singular. Because of this, it has seemed more appropriate to devise a quadrature formula which takes explicitly into account the form of the kernel functions.

To do this let $g(x)$ denote the straight line passing through (x_n,g_n), (x_{n+1},g_{n+1}),

$$g(x)=g_n+(x-x_n/h)(g_{n+1}-g_n). \tag{38}$$

Now if x' is in the interval (x_n,x_{n+1}), we have

$$\tau(x,x')=\int_{x'}^{x}\mu(x'')dx''=\int_{x'}^{x_n}\mu(x'')dx''+\int_{x_n}^{x}\mu(x'')dx''$$
$$=(x_n-x')\mu_{n+\frac{1}{2}}+\tau(x,x_n),$$

where $\mu_{n+\frac{1}{2}}$ is the (now assumed constant) value of $\mu(x)$ on the mesh interval (x_n,x_{n+1}).

Suppose $x\leqq x_n$, then

$$|\tau(x,x')|=(x'-x_n)\mu_{n+\frac{1}{2}}+\tau(x_n,x).$$

If also $l+s$ is even,

$$\int_{x_n}^{x_{n+1}}g(x')Q_{ls}(|\tau(x,x')|)dx'$$
$$=\int_{x_n}^{x_{n+1}}g(x')\left\{\int_0^1 P_l(\omega)P_s(\omega)\frac{1}{\omega}\times\exp\left[\frac{-\tau(x_n,x)-(x'-x)\mu_{n+\frac{1}{2}}}{\omega}\right]d\omega\right\}dx'$$
$$=\int_0^1 P_l(\omega)P_s(\omega)\frac{1}{\omega}\exp\left[\frac{-\tau(x_n,x)+\mu_{n+\frac{1}{2}}x_n}{\omega}\right]\times\int_{x_n}^{x_{n+1}}g(x')\exp\left[-\frac{\mu_{n+\frac{1}{2}}x'}{\omega}\right]dx'd\omega. \tag{39}$$

But from (38) we find easily

$$\int_{x_n}^{x_{n+1}}g(x')\exp\left\{-\frac{\mu_{n+\frac{1}{2}}x'}{\omega}\right\}dx'$$
$$=h\exp\left\{-\frac{x_n\mu_{n+\frac{1}{2}}}{\omega}\right\}\left\{g_n\left[\frac{\sigma_n-1+e^{-\sigma_n}}{\sigma_n^2}\right]+g_{n+1}\left[\frac{1-e^{-\sigma_n}(1+\sigma_n)}{\sigma_n^2}\right]\right\}, \tag{40}$$

where we have written

$$\sigma_n=h\mu_{n+\frac{1}{2}}/\omega. \tag{41}$$

By collecting these results, we get finally

$$\int_{x_n}^{x_{n+1}} g(x')Q_{ls}(|\tau(x_n,x')|)dx' = \alpha_{nm}g(x_n)+\beta_{nm}g(x_{n+1}), \quad (42)$$

where

$$\alpha_{nm}=\frac{1}{h\mu_{n+\frac{1}{2}}^2}\int_0^1 P_l(\omega)P_s(\omega)\omega \exp-(\tau_{nm}/\omega) \times[\sigma_n-1+e^{-\sigma_n}]d\omega$$

$$\beta_{nm}=\frac{1}{h\mu_{n+\frac{1}{2}}^2}\int_0^1 P_l(\omega)P_s(\omega)\omega \exp-(\tau_{nm}/\omega) \times[1-e^{-\sigma_n}(1+\sigma_n)]d\omega$$

$\tau_{nm}=\tau(x_n,x_m)$.

In terms of the numbers

$$\gamma_{nm}=\int_0^1 P_l(\omega)P_s(\omega)\exp-\left(\frac{|\tau_{nm}|}{\omega}\right)d\omega \quad (43)$$

$$\delta_{nm}=\int_0^1 P_l(\omega)P_s(\omega)\omega\exp-\left(\frac{|\tau_{nm}|}{\omega}\right)d\omega, \quad (44)$$

we have

$$\left.\begin{aligned}\alpha_{nm}&=\frac{1}{\mu_{n+\frac{1}{2}}}\gamma_{nm}+\frac{1}{h\mu_{n+\frac{1}{2}}^2}(\delta_{n+1,m}-\delta_{nm})\\ \beta_{nm}&=-\frac{1}{\mu_{n+\frac{1}{2}}}\gamma_{n+1,m}+\frac{1}{h\mu_{n+\frac{1}{2}}^2}(\delta_{nm}-\delta_{n+1,m})\end{aligned}\right\} \begin{array}{l} x_m\leqq x_n \quad (45)\\ l+s \\ \text{even.} \quad (46)\end{array}$$

The corresponding results for other cases are

$$\left.\begin{aligned}\alpha_{nm}&=-\frac{1}{\mu_{n+\frac{1}{2}}}\gamma_{nm}+\frac{1}{h\mu_{n+\frac{1}{2}}^2}(\delta_{n+1,m}-\delta_{nm})\\ \beta_{nm}&=\frac{1}{\mu_{n+\frac{1}{2}}}\gamma_{n+1,m}+\frac{1}{h\mu_{n+\frac{1}{2}}^2}(\delta_{nm}-\delta_{n+1,m})\end{aligned}\right\} \begin{array}{l} x_m\geqq x_{n+1} \quad (47)\\ l+s \text{ odd} \\ \text{or even} \quad (48)\end{array}$$

$$\left.\begin{aligned}\alpha_{nm}&=-\frac{1}{\mu_{n+\frac{1}{2}}}\gamma_{nm}-\frac{1}{h\mu_{n+\frac{1}{2}}^2}(\delta_{n+1,m}-\delta_{nm})\\ \beta_{nm}&=\frac{1}{\mu_{n+\frac{1}{2}}}\gamma_{n+1,m}-\frac{1}{h\mu_{n+\frac{1}{2}}^2}(\delta_{n+1,m}-\delta_{nm})\end{aligned}\right\} \begin{array}{l} x_m\leqq x_n \quad (49)\\ l+s \\ \text{odd.} \quad (50)\end{array}$$

Thus in all cases the integration coefficients of (42) may be easily obtained from the γ_{nm}, δ_{nm} of (43)–(44). These, in turn, are linear combinations of E_n functions of the matrix elements τ_{nm} and may therefore be precomputed.

A program embodying the methods given in this paper is now in preparation at the Argonne National Laboratory, and a report on the results obtained with it will be made at a future date.

Double Commutator in Quantum Field Theory*

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A representation is obtained for the most general function with the properties of the double commutator, including nonzero mass thresholds but not the Jacobi identities. The thresholds are proved to satisfy triangular inequalities (without using any more information) which are always true physically. The problem of incorporating a discrete level at the mass of a stable particle is not solved.

IN a previous paper[1] we have obtained an integral representation for the double commutator $D(x,y) = \langle 0|[A(x_1),[B(x_2),C(x_3)]]|0\rangle$, where $x=x_1-x_2$, $y=x_2-x_3$, and A, B, C are local fields. More exactly, the following theorem was proved:

Suppose $D(x,y)$ has the properties (1), (2), (3), (4): (1) $D(x,y)$ is Lorentz invariant; (2) $D(x,y) = D(-x,-y)$; (3) $\tilde{D}(p,q)=0$, unless p, q are timelike or $p, p-q$ timelike; (4) $D(x,y)=0$, if $y^2<0$; Then $D(x,y)$ has the representation

$$D(x,y)=\int_0^\infty \theta[\lambda-(st)^{\frac{1}{2}}]\phi(s,t,\lambda;k) \times \Delta_2(x, x+y; s,t,\lambda)\Delta(y;k)ds dt d\lambda dk \quad (5)$$

for at least one ϕ. In (5)

$$\Delta_2(x,y;s,t,\lambda) = \int e^{-ipx-iqy}\delta(p^2-s)\delta(p\cdot q-\lambda)\delta(q^2-t)\epsilon(p_0)d^4p d^4q.$$

The form (5) also has the additional property[2]

$$D(x,y)=0, \text{ if } x \text{ and } x+y \text{ are space-like.} \quad (6)$$

Equation (6) therefore follows from (1)–(4), a result found by Symanzik,[3] which is closely connected with analytic completion. The functions ABC, ACB, $\cdots$, which make up D have some analytic properties,[1] which follow from (1), (2), (3), (4), leading to a result like (6).

Now we are interested in putting more information into the condition (3), namely, the knowledge of the thresholds of the mass spectra. Of the terms in the double commutator, ABC and CBA are zero unless $p^2 \geqslant m_1^2$, $q^2 \geqslant m_3^2$, and ACB, BCA are zero unless $p^2 \geqslant m_1'^2$, $(p-q)^2 \geqslant m_2^2$. We have given m_1 and m_1' different symbols, but later we prove that they must be the same. The masses are defined as

$$m_1^2 = \min\gamma^2 \text{ such that } \langle 0|A|\gamma\rangle\langle\gamma|BC|0\rangle \neq 0 \quad (7)$$

$$m_1'^2 = \min\gamma^2 \text{ such that } \langle 0|A|\gamma\rangle\langle\gamma|CB|0\rangle \neq 0 \quad (8)$$

$$m_3^2 = \min\gamma^2 \text{ such that } \langle 0|AB|\gamma\rangle\langle\gamma|C|0\rangle \neq 0 \quad (9)$$

$$m_2^2 = \min\gamma^2 \text{ such that } \langle 0|AC|\gamma\rangle\langle\gamma|B|0\rangle \neq 0. \quad (10)$$

If A, B, and C are fields of particles, there will perhaps be discrete levels at these masses, the spectrum being zero again until the threshold of the continuum. We cannot deal with this property simply, and so ignore it. If A, B, C are local currents there is no discrete level. It is an interesting question whether derivability from a field places any restriction on the current. We take A, B, C to be local currents, and so replace (3) by

$$\tilde{D}(p,q)=0 \quad \text{unless} \quad \begin{cases} p^2 \geqslant m_1^2,\ q^2 \geqslant m_3^2, \text{ or} \\ p^2 \geqslant m_1'^2,\ (p-q)^2 \geqslant m_2^2 \end{cases} \quad (11)$$

$$\tilde{D}(p,q) \neq 0 \quad (12)$$

in this spectrum.

It is conceivable that the properties (1), (2), (4), and (11) already imply that $\tilde{D}(p,q)$ vanishes in a region larger than (12). We shall show that (12) is inconsistent with (1), (2), (4), and (11) unless

$$m_1 = m_1' \quad (13)$$

$$m_2 \leqslant m_3+m_1; \quad m_3 \leqslant m_1+m_2. \quad (14)$$

Similarly, by using another commutator $[C[A,B]]$ we could prove

$$m_1 \leqslant m_2+m_3. \quad (15)$$

This result is connected with a type of theorem first proved by Dyson,[4] namely, that it is not possible to construct functions with arbitrary support and spectra.

Equations (13), (14), and (15) can be shown easily using some further properties usually ascribed to the fields and Hilbert space, but then it is not obvious exactly what information is being used. For example, if $\langle\gamma_1|AC|0\rangle \neq 0$, then $\langle\gamma_1|CA|0\rangle \neq 0$; any $|\gamma\rangle$ occurring in (7) also occurs in (8), and vice versa. This proves (13). To prove (15) note that if $|\gamma_2\rangle$ and $|\gamma_3\rangle$ are such that $\langle 0|B|\gamma_2\rangle \neq 0$ and $\langle 0|C|\gamma_3\rangle \neq 0$, then they also satisfy $\langle 0|AC|\gamma_2\rangle \neq 0$ and $\langle 0|AB|\gamma_3\rangle \neq 0$ (given that

* Part of work submitted for the Ph.D. degree at the University of London.

[1] R. F. Streater, "Special methods of analytic completion in field theory," Proc. Roy. Soc. (London) (to be published).

[2] R. F. Streater, thesis, London 1959 (unpublished); "Some integral representations in field theory," Nuovo cimento 15, 937 (1960).

[3] K. Symanzik (private communication).

[4] F. J. Dyson, Phys. Rev. 110, 1460 (1958).

ABC is not identically zero). Then the state $|\gamma_2,\gamma_3\rangle$ has the same quantum numbers as A. By $|\gamma_2,\gamma_3\rangle$ we mean the state obtained by adding the particles in state $|\gamma_2\rangle$ to those in $|\gamma_3\rangle$: $|\gamma_2,\gamma_3\rangle = |\gamma_2\rangle \wedge |\gamma_3\rangle$.[5] These particles can form a state with γ_2 and γ_3 parallel to each other. We can also find a state $|\gamma_2\rangle$ such that $\gamma_2^2 = m_2^2$, and a state $|\gamma_3\rangle$ such that $\gamma_3^2 = m_3^2$, in which case $|\gamma_2,\gamma_3\rangle$ has mass m_2+m_3 and satisfies $\langle 0|A|\gamma_2,\gamma_3\rangle \neq 0$. Hence $|\gamma_2,\gamma_3\rangle$ is a state $|\gamma\rangle$ occurring in (7), and so $m_1 \leqslant m_2+m_3$. Similarly, the other inequalities (14) can be proved. This argument has been given to show the physical meaning of (13), (14) and (15); a mathematical proof is given below.

If A, B, and C are fields, the inequalities (14) and (15) do not imply that they must describe stable particles; m_1, m_2, and m_3 are not necessarily the "masses" of the fields A, B, and C. This is because the lowest state connected to the field need not be a one-particle state (and cannot be if the field describes an unstable particle). The inequalities (14) will be needed below in the method adopted to include the mass-spectrum (11) into the representation (5). It is therefore of interest that (13), (14) follow from (1), (2), (4), (11), and (12) without using the arguments about Hilbert space.

Proof of (13)

Consider $\theta(p_0)\bar{D}(p,q)$. This is zero unless $p^2 \geqslant m_1^2$ and $q^2 \geqslant m_3^2$, $q_0>0$, or $p^2 \geqslant m_1'^2$, $(p-q)^2 \geqslant m_2^2$, $p_0 > q_0$, and so may be decomposed (nonuniquely) into two functions $\langle ABC\rangle_{\rm av}(p,q) - \langle ACB\rangle_{\rm av}(p,q)$ such that

$$\langle ABC\rangle_{\rm av}(p,q)=0, \quad \text{unless} \quad p^2 \geqslant m_1^2,\ q^2 \geqslant m_3^2;\ p_0,\ q_0>0.$$

$$\langle ACB\rangle_{\rm av}(p,q)=0, \quad \text{unless} \quad p^2 \geqslant m_1'^2,\ (p-q)^2 \geqslant m_2^2;\ p_0,\ p_0-q_0>0$$

and

$$\int \langle ABC\rangle_{\rm av}(p,q)e^{-iqy}dq^4 = \int \langle ACB\rangle_{\rm av}(p,q)e^{-iqy}dq^4 \quad \text{if} \quad y^2<0 \qquad (16)$$

by using (4).

Then if $p^2 < \max(m_1^2, m_1'^2)$, one or other side of (16) is identically zero as a function of y. For a given p, $ABC(p,y)$ is regular in the backward tube $\mathrm{Im}\, y<0$, and $ACB(p,y)$ is regular in the forward tube $\mathrm{Im}\, y>0$, as is seen by examining their spectra in q. But by (16) they are equal when $y^2<0$. Using the "Edge of the Wedge" theorem[6] they continue one another and are regular for the points $y^2<0$. If either side of (16) is zero for $y^2<0$ it must be zero everywhere, and so must the other side. So both sides are zero unless $p^2 \geqslant \max(m_1^2, m_1'^2)$ and in order to avoid a contradiction with (12) we must have $m_1 = m_1'$.

[5] W. Brennig and R. Haag, Fortschr. Physik 7, 183 (1959).
[6] H. J. Bremmerman, R. Oehme, and J. G. Taylor, Phys. Rev. 109, 2178 (1958).

To prove (14) we apply Dyson's lemma[4] to the function $\tilde{f}(p,q) = \theta(p_0)\bar{D}$. Because of (4), $\tilde{f}$ has the representation

$$\tilde{f}(p,q) = \int \phi(p,u,k)\delta((q-u)^2-k^2)\epsilon(q-u)d^4u dk^2, \qquad (17)$$

where $\phi(p,u,k)=0$, unless $p>0$, and unless the hyperbola in q space for fixed (u,k) given by

$$(q-u)^2 = k^2 \qquad (18)$$

lies *entirely* in the spectrum of $\tilde{f}(p,q)$. The hyperbola (18) has two branches, one with $q_0 \to \infty$ and the other with $q_0 \to -\infty$. The first branch must lie entirely in p, $q>0$ and the second entirely in p, $p-q>0$ (the sign >0 means "lies in the forward light cone"). Now $q=(q-u)+u$, and to be >0 for all $q-u$ on the positive branch of (18) we must have $u>0$. Since $q^2 = (q-u)^2 + 2u\cdot(q-u)+u^2$, we have

$$q^2 \geqslant k^2 + 2k(u^2)^{\frac{1}{2}} + u^2 \qquad (19)$$

(q on the positive branch). Equality can be obtained in (19) for some q of (18). So if the positive branch of (18) is to lie in the set $q^2 \geqslant m_3^2$, $q_0>0$ for all q, we must have

$$k^2 + 2k(u^2)^{\frac{1}{2}} + u^2 \geqslant m_3^2. \qquad (20)$$

We also require that the negative branch of (18) should lie in the set $(p-q)^2 \geqslant m_2^2$, $p_0 > q_0$. Now $p-q = (p-u)-(q-u)$, and is forward timelike for all $q-u$ on the negative branch of (18) only if $p-u>0$. Then using $(p-q)^2 = (p-u)^2 - 2(p-u)\cdot(q-u)+k^2$, we get

$$(p-q)^2 \geqslant (p-u)^2 + 2k[(p-u)^2]^{\frac{1}{2}} + k^2 \qquad (21)$$

(q on the negative branch) equality in (21) holding for some points of (18). Thus to ensure $(p-q)^2 \geqslant m_2^2$ we require

$$(p-u)^2 + 2k[(p-u)^2]^{\frac{1}{2}} + k^2 \geqslant m_2^2. \qquad (22)$$

If we solve (20) and (22) for k, we get

$$k \geqslant m_3 - [u^2]^{\frac{1}{2}} \qquad (23)$$

$$k \geqslant m_2 - [(p-u)^2]^{\frac{1}{2}}. \qquad (24)$$

Therefore we have shown that ϕ in (17) can be chosen zero unless $p>0$, $u>0$, $p-u>0$ and $k \geqslant \max\{0;\ m_3-[u^2]^{\frac{1}{2}};\ m_2-[(p-u)^2]^{\frac{1}{2}}\}$. Because of (19) and (21), the spectrum will be *too small* unless both the extrema of k ($m_3-[u^2]^{\frac{1}{2}}$ and $m_2-[(p-u)^2]^{\frac{1}{2}}$), are attained for some u. Thus the condition that $\tilde{f}(p,q)$ is nonzero when $q^2=m_3^2$ and $(p-q)^2=m_2^2$ imposes the inequalities

$$m_3 - [u^2]^{\frac{1}{2}} \geqslant m_2 - [(p-u)^2]^{\frac{1}{2}} \qquad (25)$$

for some u such that $p>u>0$,

$$m_2 - [(p-u)^2]^{\frac{1}{2}} \geqslant m_3 - [u^2]^{\frac{1}{2}} \qquad (26)$$

for some u such that $p>u>0$.

The best case of (25) is when $u=0$, and of (26) is $u=p$, giving

$$m_3 \geqslant m_2 - [p^2]^{\frac{1}{2}}$$
$$m_2 \geqslant m_3 - [p^2]^{\frac{1}{2}}.$$

If $p^2=m_1^2$ is a value of p, where $\bar{f}(p,q)\neq 0$, we get the inequalities (14). To sum up, causality imposes triangular inequalities on the thresholds of the spectra of three fields if their product has nonzero expectation value.

If we impose Lorentz invariance on (17), we see that $\phi(u,p,k)$ can be chosen as a Lorentz invariant function zero, unless $u, p-u>0$ and $p^2 \geqslant m_1^2$. In general this has the form

$$\phi(u,p,k)=\int_0^\infty \psi(s,t,\lambda;k)\delta(u^2-s)\delta(u(p-u)-\lambda) \times\delta((p-u)^2-t)\theta(u_0)dsdtd\lambda. \quad (27)$$

Since $p^2=(p-u)^2+u^2+2u\cdot(p-u)$, a ψ can be chosen zero if $\lambda<\frac{1}{2}(m_1^2-s-t)$. Finally, by using (2), we get for the double commutator the representation (5), with the limits of integration

$$\begin{gathered} s, t>0 \\ \lambda \geqslant \max([st]^{\frac{1}{2}}; \tfrac{1}{2}(m_1^2-s-t)) \\ k \geqslant \max(0; m_2-t; m_3-s). \end{gathered} \quad (28)$$

The author has proposed[2] integral representations for triple commutators, without the proof that they give the most general function. In the same way as in the present paper it is possible to incorporate the mass-spectrum provided certain inequalities are satisfied by the thresholds. It is worth noting that all these inequalities are satisfied in practice.

Some Remarks Concerning the Real and Imaginary Parts of the Characteristic Roots of a Finite Matrix

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Some theorems are obtained on the existence of certain determinantal equations whose roots are separately the real or imaginary parts of the characteristic roots of a given matrix with simple elementary divisors. When the elementary divisors are not simple, similar, but somewhat less precise, results are obtained.

THE purpose of this paper is to generalize some previously known theorems on the real parts of the characteristic roots of a finite real matrix (cf. footnote references 2 and 5), to refine their proofs by presenting them from a unified point of view, and to show that the same methods yield similar results concerning the imaginary parts of the roots. Also, analogous results for complex matrices are indicated.

In the sequel we use the following notation: If X is a matrix, $\bar{X}$ is the conjugate complex of X, X' is the transpose of X, and $X^*=\bar{X}'$.

THEOREM 1

Given any (not necessarily real) matrix A of order n with simple elementary divisors and with characteristic roots, $\alpha_1, \cdots, \alpha_n$. Then it is always possible to find a positive definite Hermitian matrix G (of order n) such that the roots $\lambda_1, \cdots, \lambda_n$ of the equation $\det(\sigma GA+\bar{\sigma}A^*G-2\lambda G)=0$ are the real parts of $\sigma\alpha_1, \cdots, \sigma\alpha_n$, where σ is any complex number and $\bar{\sigma}$ is its conjugate complex. Moreover, if A is real, G may be chosen so as to be real also. In any case, G is independent of σ.

Proof

Since the matrix A is similar to a diagonal matrix, we have

$$S^{-1}AS=\text{diagonal } (\alpha_1,\cdots,\alpha_n)$$

for some suitably chosen nonsingular matrix S. Hence

$$S^{-1}\sigma AS=\text{diagonal } (\sigma\alpha_1,\cdots,\sigma\alpha_n),$$
$$S^*\bar{\sigma}A^*S^{*-1}=\text{diagonal } (\bar{\sigma}\bar{\alpha}_1,\cdots,\bar{\sigma}\bar{\alpha}_n).$$

Hence $\frac{1}{2}(S^{-1}\sigma AS+S^*\bar{\sigma}A^*S^{*-1})$ has as characteristic roots the real parts of the $\sigma\alpha_i$. This latter matrix is equal to

$$\tfrac{1}{2}S^*(\sigma S^{*-1}S^{-1}ASS^*+\bar{\sigma}A^*)S^{*-1},$$

which is similar to $\frac{1}{2}(\sigma GAG^{-1}+\bar{\sigma}A^*)$, if we put $SS^*=G^{-1}$. But the statement that $\frac{1}{2}(\sigma GAG^{-1}+\bar{\sigma}A^*)$ has the real parts of the $\sigma\alpha_i$ as its characteristic roots is equivalent to the statement to be proved about the roots of the above-mentioned determinantal equation in λ. The fact that $G=S^{*-1}S^{-1}$ is positive definite, Hermitian, and independent of σ is obvious. To show that G can be chosen to be real when A is real, we observe that S has as its columns the characteristic vectors of A. These characteristic vectors can be chosen real for real characteristic roots and conjugate complex for a pair of conjugate complex roots. It follows that $\bar{S}=SE$ where E is a permutation matrix which is a direct sum of a unit matrix and matrices of the form

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}.$$

Hence E is symmetric. We then have $S^*=ES'$. Hence $SS^*=SES'=\bar{S}S'$ and $(SS^*)'=S\bar{S}'=SS^*$. Since $G^{-1}=SS^*$ is Hermitian and symmetric, it must be real.[1]

Corollary 1.1

Given any real matrix A with simple elementary divisors, it is always possible to find a positive definite symmetric matrix G (of the same order as A) such that the roots $\lambda_1, \cdots, \lambda_n$ of the equation $\det(B-2\lambda G)=0$, where $B=GA+A'G$, are the real parts of the characteristic roots of A.

This is deduced immediately from Theorem 1 by taking $\sigma=1$.

This result was first stated and proved by Lewis[2] with the unnecessary restriction that A be nonsingular. The proof there given was based on concepts of tensor analysis instead of the purely matrix methods of the present paper.

Corollary 1.2

The positive definite symmetric matrix G of Corollary 1.1 may be chosen so as not only to satisfy the conditions of that corollary but so that simultaneously the roots of the equation $\det(C-2\lambda G)=0$, where $C=GA-A'G$, are the

[1] An alternative proof would have been to replace every pair of complex conjugate elements in diagonal $(\alpha_1,\cdots,\alpha_n)$ by the real matrix

$$\begin{pmatrix}R\alpha & I\alpha\\ -I\alpha & R\alpha\end{pmatrix}.$$

[2] D. C. Lewis, Am. J. Math. 73, 48 (1951).

imaginary parts, multiplied by $\sqrt{-1}$, of the characteristic roots of A.

This is deduced from Theorem 1 by taking $\sigma=\sqrt{-1}$, with emphasis on the fact that the G of Theorem 1 is independent of σ.

Corollary 1.3

The matrix B of Corollary 1.1 has the same signature as the real parts of the characteristic roots of A.

This follows from the fact that the signature of the roots of $\det(B-2\lambda G)=0$ is the same as the signature of the characteristic roots of BG^{-1}, which latter matrix is similar to $G^{-\frac{1}{2}}BG^{-\frac{1}{2}}$, which has the same signature as B.

Remark

Corollary 1.1 (and hence Theorem 1) ceases to be true if the hypothesis about the simple elementary divisors is omitted. As an example take

$$A=\begin{pmatrix}1 & 1\\ 0 & 1\end{pmatrix}.$$

If

$$G=\begin{pmatrix}a & b\\ b & c\end{pmatrix},$$

which is the most general symmetric matrix of order two, we find that

$$B=GA+A'G=\begin{pmatrix}2a & a+2b\\ a+2b & 2b+2c\end{pmatrix}.$$

We now find easily enough that $\det(GA+A'G-2\lambda G)=0$ has a root $\lambda=1$ if and only if

$$\begin{vmatrix}0 & a\\ a & 2b\end{vmatrix}=0, \quad \text{or} \quad a=0.$$

Hence G cannot be positive definite, as required by the Corollary.

We are, however, able to state the following theorem in which A is not required to have simple elementary divisors.

THEOREM 2

Given any (not necessarily real) matrix A of order n with characteristic roots, $\alpha_1, \cdots, \alpha_n$. Given also a positive number ϵ. Then it is always possible to find a positive definite Hermitian matrix G (of order n) such that the roots $\lambda_1, \cdots, \lambda_n$ of the equation $\det(\sigma GA+\bar{\sigma}A^*G-2\lambda G)=0$ are real and differ from the real parts of $\sigma\alpha_1, \cdots, \sigma\alpha_n$ by not more than $|\sigma|\epsilon$, where σ is any complex number. Moreover, if A is real, G may be chosen so as to be real also. In any case, G, though dependent on A and ϵ, is independent of σ.

The proof is a modification of the proof of Theorem 1. Let S be a matrix which transforms A into a modified Jordan canonical form J_ϵ:

$$S^{-1}AS=J_\epsilon,$$

where J_ϵ consists of a diagonal containing the characteristic roots of A and a superdiagonal containing 0's and ϵ's. All other elements of J_ϵ are 0. As in Theorem 1, if we set $G=(SS^*)^{-1}$ we find that the matrix $\frac{1}{2}(G\sigma AG^{-1}+\bar{\sigma}A^*)$ is similar to a Hermitian matrix K whose elements are all 0, except for the diagonal, which contains the real parts of the numbers $\sigma\alpha_1, \cdots, \sigma\alpha_n$, and for some of the elements in the super- and subdiagonal which are equal to $\sigma\epsilon/2$ and $\bar{\sigma}\epsilon/2$, respectively. Since K splits up into blocks with equal elements on the diagonal, it follows that any characteristic root of K must differ from some one of the real parts of the numbers $\sigma\alpha_1, \cdots, \sigma\alpha_n$ by a quantity x which satisfies the equation

$$\begin{vmatrix} x & \sigma\epsilon/2 & 0 & 0 & \cdots\\ \bar{\sigma}\epsilon/2 & x & \sigma\epsilon/2 & 0 & \cdots\\ 0 & \bar{\sigma}\epsilon/2 & x & \sigma\epsilon/2 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \end{vmatrix}=0,$$

where the determinant on the left contains a suitable number of rows. It can be proved that $|x|\leqq|\sigma|\epsilon$. This follows from the Gersgorin-Brauer theorem.[3]

Furthermore, if A is real, S can be chosen so that SS^* is real. This follows in a way analogous to the corresponding part of the proof of Theorem 1, only here the matrix is built up from the so-called "principal vectors" which correspond to the characteristic roots. These have been studied by Wielandt.[4]

Corollary 2.1

Given any real matrix A and a positive number ϵ, it is always possible to find a positive definite symmetric matrix G such that the roots $\lambda_1, \cdots, \lambda_n$ of the equation $\det(B-2\lambda G)=0$, where $B=GA+A'G$, differ from the real parts of the characteristic roots of A by not more than ϵ.

This follows from Theorem 2 by taking $\sigma=1$.

Corollary 2.2

The positive definite symmetric matrix G of Corollary 2.1 may be chosen so as not only to satisfy the conditions of that corollary but so that simultaneously the roots of the equation $\det(C-2\lambda G)=0$, where $C=GA-A'G$, are pure imaginary and differ from the imaginary parts, multiplied by $\sqrt{-1}$, of the characteristic roots of A by quantities which in absolute value do not exceed ϵ.

This is deduced from Theorem 2 by taking $\sigma=\sqrt{-1}$, with emphasis on the fact that the G of Theorem 2 is independent of σ.

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[3] O. Taussky, Am. Math. Monthly **56**, 672 (1949).

[4] R. Zurmühl, *Matrizen* (Springer–Verlag, Berlin, 1950), pp. 211–226.

Corollary 2.3

If the real parts of the characteristic roots of A are all different from zero, the matrix B of Corollary 2.1 has the same signature as the real parts of the characteristic roots of A, provided that $\epsilon <$ minimum of the absolute value of the real parts of the characteristic roots of A.

This follows from the fact that the signature of the roots of $\det(B-2\lambda G)=0$ is the same as the signature of the characteristic roots of BG^{-1}, which latter matrix is similar to $G^{-\frac{1}{2}}BG^{-\frac{1}{2}}$, which has the same signature as B.

This theorem was first discovered by Bass.[5] If some of the real parts of the characteristic roots are zero then it is not always possible to find a positive definite G such that $AG+GA'$ has the same signature as the real parts of the roots of A.

In all six corollaries we have restricted attention to real matrices A. But, of course, they can all be modified to hold for complex matrices A, if we are willing to accept G as a Hermitian matrix instead of insisting that it be real and symmetric.

[5] R. W. Bass, (to be published).

Decomposition of Direct Products of Representations of the Inhomogeneous Lorentz Group

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The direct products of the physically significant, irreducible, unitary representations of the proper, orthochronous inhomogeneous Lorentz group are reduced. It is shown that $\Gamma m_1 s_1 \otimes \Gamma m_2 s_2$ contains only irreducible components of the form Γ_{mJ}, and that Γ_{mJ} occurs with nonzero multiplicity only if $J-(s_1+s_2)$ is an integer. For such J's the multiplicity of $\Gamma_{m,J}$ for $J \geq s_1+s_2$ is $(2s_1+1)(2s_2+1)$ for each positive m. $\Gamma m_1 s_1 \otimes \Gamma s_2{}^{(\pm)}$ contains only irreducible components of the form Γ_{mJ}, where $J-(s_1+s_2)$ is an integer. The multiplicity of such $\Gamma_{m,J}$ for $J \geq s_1+s_2$ is $(2s_1+1)$ for each positive m. $\Gamma s_1{}^{(\epsilon_1)} \otimes \Gamma s_2{}^{(\epsilon_2)}$ contains irreducible components of the form $\Gamma_s{}^{(\epsilon)}$ and Γ_{mJ}, where $s=|\epsilon_1 s_1+\epsilon_2 s_1|$, $\epsilon=\text{sign}\ (\epsilon_1 s_1+\epsilon_2 s_2)$ and $J-(s_1+s_2)$ is an integer. The multiplicity of $\Gamma_{m,J}$ is one for $J \geq (s_1+s_2)$ and for each positive m. The multiplicity of $\Gamma_s{}^{(\epsilon)}$ is infinite. The symmetrized squares are also analyzed. Numerous examples are given.

I. INTRODUCTION

THE famous Clebsch-Gordan rule for reducing direct (or Kronecker) products of irreducible representations of the three-dimensional rotation group has proved extremely useful in the treatment of angular momentum and in the theory of atomic spectra. It now appears that some analogous rules for the reduction of direct products of irreducible representations of the inhomogeneous Lorentz groups would be useful in the study of elementary particle physics. This article will be devoted to the derivation of such rules for the proper, orthochronous, inhomogeneous Lorentz group.[1]

Following are some examples of physical questions which are answered by the subsequent group-theoretic analysis[2]:

1. Given two relativistic particles of nonvanishing rest masses m_1 and m_2, and spins s_1 and s_2, what are the possible values of the energy in the center of mass frame (frame in which the total momentum 3 vector is zero), and of the total angular momentum for each such energy?

2. Ditto, in case one particle has zero mass and helicity λ, or both particles have zero mass and given helicities, for those states in which a center of mass frame exists.

3. In the exceptional case where no center of mass frame exists, namely those states in which two zero mass particles have parallel momenta, what are the possible values of the helicity?

4. Which of the foregoing values become inaccessible if the two particles are identical and satisfy either Bose-Einstein or Fermi-Dirac statistics?

The basis of the generalized Clebsch-Gordan decomposition rules to be derived here is the Mautner theorem[3] which states that every unitary representation of "practically" every locally compact group can be expressed as the direct integral[4] of irreducible unitary representations. Since the Mautner theorem applies to the inhomogeneous Lorentz group, and since the direct product of two unitary representations is a unitary representation, it follows that the direct product of two irreducible unitary representations of the inhomogeneous Lorentz group can be expressed as the direct integral of irreducible unitary representations. The Mautner theorem, however, does not guarantee the uniqueness of the direct integral decomposition. Uniqueness is guaranteed if the group is of type **I**,[5] and it can be shown from some theorems due to Mackey[6] that the proper, orthochronous, inhomogeneous Lorentz group is of type I. The physically significant irreducible unitary representations of the inhomogeneous Lorentz group were found by Wigner,[7] and these are the only ones that will be considered here.

Since a rigorous mathematical treatment of this reduction problem would require a considerable amount of advanced analysis and epsilonics, the problem will be treated here in a rather naive way. In particular, the direct integrals will be treated as direct sums, so what will be found are just the irreducible component representations of the direct products.

[1] Some of the results to be derived here have already been obtained for special cases by L. Michel, page 272 of the multigraphed report, "Congres international sur le rayonnement cosmique, organisè par l'Université Toulouse," sous le Patronage de l'UIPPA avec la UNESCO, July, 1953; Bagneres de Bigorre and E. P. Wigner, Nuovo cimento **3**, 517 (1956).

[2] I am indebted to the referee for suggesting the inclusion of these problems.

[3] F. I. Mautner, Ann. Math. **51**, 1 (1950); **52**, 8 (1950). See also M. A. Naimark and S. V. Fomin, Am. Math. Soc. Translations **5**, 35 (1957).

[4] The direct integral of representations is a generalization of the direct sum. See Naimark and Fomin, footnote reference 3.

[5] G. W. Mackey, "Theory of group representations" (Mimeographed Notes, Department of Mathematics, University of Chicago, 1955).

[6] G. W. Mackey, Acta Math. **99**, 265 (1958).

[7] E. P. Wigner, Ann. Math. **40**, 149 (1939). See also Iu. M. Shirokov, Soviet Phys. JETP **6**, 664, 919, 929 (1958); V. Bargmann and E. Wigner, Proc. Natl. Acad. Sci. **34**, 211 (1948); T. S. Chang, Acta Math. Sinica **3**, 59 (1953); L. L. Foldy, Phys. Rev. **102**, 568 (1956); C. Fronsdal, *ibid.* **113**, 1367 (1959); J. S. Lomont, *Applications of Finite Groups* (Academic Press Inc., New York, 1959), Appendix III; and G. W. Mackey, footnote reference 5, p. 171.

The technique which will be employed is to reduce the problem to a reduction problem for the rotation group and then to apply the idempotent method which was applied by Jacob and Wick[8] to scattering theory.

II. REVIEW OF REPRESENTATIONS[9]

The irreducible unitary representations of the proper, orthochronous, inhomogeneous Lorentz group to be considered here are all infinite-dimensional

The proper, orthochronous, inhomogeneous Lorentz group[10] is the set of all ordered pairs $(L|a)$, where L is a real 4×4 matrix satisfying the three conditions

$$L^tGL=G \quad G=\begin{bmatrix}-1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix} \tag{2.1}$$

$$\det(L)=1 \tag{2.2}$$

$$\text{upper left element of } L\geq 0, \tag{2.3}$$

where a is any real four-dimensional column matrix, and multiplication is defined by

$$(L|a)(L'|a')=(LL'|La'+a). \tag{2.4}$$

The irreducible unitary representations[11] to be considered here are of two types and will be denoted by $\Gamma_{m,s}$ and $\Gamma_s^{(\pm)}$, where $0<m<\infty$, $s=0, \frac{1}{2}, 1, \frac{3}{2}\cdots$. The reps $\Gamma_{m,s}$ belong to mass m and spin s, while the reps $\Gamma_s^{(\pm)}$ belong to mass zero, spin s, and spin parallel or antiparallel to momentum.

Let $\Gamma=\{D[(L|a)]\}$ be a unitary representation of $\mathfrak{IL}$ and let the operator corresponding to the infinitesimal transformation $(L|a)$ given by

$$L=\|L^\mu{}_\nu\|, \quad L^\mu{}_\nu=\delta^\mu{}_\nu+\omega^{\mu\nu}g_{\lambda\nu}\,\omega^{\mu\nu}=-\omega^{\nu\mu}, \tag{2.5}$$

and infinitesimal a^μ be

$$D[(L|a)]=I+(i/2)\omega^{\mu\nu}J_{\mu\nu}+ia^\lambda P_\lambda. \tag{2.6}$$

The 10 operators $P_\lambda, J_{\mu\nu}$ satisfy the commutation relations

$$[P_\kappa,P_\lambda]_-=0 \tag{2.7}$$

$$[P_\lambda,J_{\mu\nu}]_-=ig_{\lambda\nu}P_\mu-ig_{\lambda\mu}P_\nu \tag{2.8}$$

$$[J_{\kappa\lambda},J_{\mu\nu}]_-=ig_{\kappa\mu}J_{\lambda\nu}+ig_{\lambda\nu}J_{\kappa\mu}-ig_{\kappa\nu}J_{\lambda\mu}-ig_{\lambda\mu}J_{\kappa\nu}. \tag{2.9}$$

Consequently, if one lets

$$C_1=-P^\lambda P_\lambda \tag{2.10}$$

$$C_2=-\tfrac{1}{2}J^{\lambda\mu}J_{\lambda\mu}P^\nu P_\nu+J^{\lambda\mu}J_{\lambda\nu}P^\nu P_\mu, \tag{2.11}$$

one finds that the two operators C_1 and C_2 commute with the 10 operators $P_\lambda, J_{\mu\nu}$. These two operators are called Casimir operators and in a rep must be scalar operators. Thus in Γ_{ms}, $C_1=m^2$, $C_2=m^2s(s+1)$; and in $\Gamma_s^{(\pm)}$, $C_1=C_2=0$. If one lets

$$v_{\lambda\mu\nu}=-iP_\lambda J_{\mu\nu}-iP_\mu J_{\nu\lambda}-iP_\nu J_{\lambda\mu} \tag{2.12}$$

$$w_\lambda=(v_{123},v_{230},v_{310},v_{012}), \tag{2.13}$$

then one can distinguish the massless reps by the fact that

$$w_\lambda=\mp\text{is } P_\lambda \quad \text{in } \Gamma_s^{(\pm)}.$$

The Bargmann-Wigner construction of $\Gamma_{m,s}$ is as follows. Let p_λ be any set of four real numbers satisfying $p^\lambda p_\lambda=-m^2$ (m fixed) and $p^0\geq0$; and let $\psi(p_\lambda)$ be any solution of the equation

$$(\gamma^\lambda p_\lambda-im)=0, \quad p^0>0, \tag{2.14}$$

where the γ's are 4×4 Dirac matrices satisfying

$$[\gamma^\mu,\gamma^\nu]_+=2g^{\mu\nu}. \tag{2.15}$$

Then the carrier (or representation) space $H_{m,\frac{1}{2}}$ for $\Gamma_{m,\frac{1}{2}}$ is the set of all solutions $\psi(p_\lambda)$ of (2.14) with a finite norm, defined by

$$\|\psi\|^2=\int\psi^+\beta\psi\frac{d^{(3)}p}{|(|\mathbf{p}|^2+m^2)^{\frac{1}{2}}|}, \tag{2.16}$$

where $\beta=i\gamma^0$ and $p^0=+(|\mathbf{p}|^2+m^2)^{\frac{1}{2}}$. The carrier space $H_{m,s}$ for $s>\frac{1}{2}$ is[12] defined as the symmetric subspace of the $2s$th Kronecker power with respect to spin indices of $H_{m,\frac{1}{2}}$ with norm defined by

$$\|\psi\|^2=\int\psi^+\beta_1\beta_2\cdots\beta_{2s}\psi\frac{d^{(3)}p}{|(|\mathbf{p}|^2+m^2)^{\frac{1}{2}}|}, \tag{2.17}$$

where $\beta_j=I\otimes I\otimes\cdots\otimes I\otimes\beta\otimes I\otimes\cdots\otimes I$, I is the 4×4 unit matrix, and β is in the jth position. The inner product is defined by the equation

$$\begin{aligned}\langle\phi|\psi\rangle\equiv&-\tfrac{1}{4}\{\|\psi-\phi\|^2-\|\psi+\phi\|^2\\&+i\|\psi-i\phi\|^2-i\|\psi-+i\phi\|^2\}\\=&\int\phi^+\beta_1\beta_2\cdots\beta_{2s}\psi\frac{d^{(3)}p}{|(|\mathbf{p}|^2+m^2)^{\frac{1}{2}}|}.\end{aligned} \tag{2.18}$$

The operators P_λ and $J_{\mu\nu}$ are defined in $H_{m,s}$ by

$$P_\lambda\psi(p)=p_\lambda\psi(p) \tag{2.19}$$

$$J_{\mu\nu}=M_{\mu\nu}+S_{\mu\nu} \tag{2.20}$$

$$M_{\mu\nu}=-i\{[p_\mu(\partial/\partial p^\nu)]-[p_\nu(\partial/\partial p^\mu)]\}^{13} \tag{2.21}$$

$$S_{\mu\nu}=-\frac{i}{4}\sum_{u=1}^{2s}[\gamma_{nu},\gamma_{n\nu}]_-. \tag{2.22}$$

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[8] M. Jacob and G. C. Wick, Ann. Physics 7, 404 (1959).

[9] We put $\hbar=c=1$, $-g_{00}=g_{11}=g_{22}=g_{33}=1$. Latin indices run from 1 to 3, Greek indices from 0 to 3. * means complex conjugate, and † means adjoint or Hermitian conjugate.

[10] The proper orthochronous inhomogeneous Lorentz group will subsequently be referred to as $\mathfrak{IL}$.

[11] Irreducible unitary representations will subsequently be called reps.

[12] For $s=0$ there is no equation and the wave function ψ has a single component.

[13] To calculate $M_{\mu\nu}\psi$, express ψ as a function of p_μ, p_ν, and one

The construction of $\Gamma_s^{(\pm)}$ is the same, except that $m=0$ and that ψ must satisfy the additional condition

$$\gamma_n{}^5\psi=\pm\psi \text{ for } \Gamma_s^{(\pm)}, \tag{2.23}$$

where

$$\gamma_n{}^5=i\gamma_{n0}\gamma_{n1}\gamma_{n2}\gamma_{n3}. \tag{2.24}$$

The spinless representation is obtained from Γ_{m0} by putting $m=0$.

The following properties of representations of $\mathfrak{IL}$ will be useful in the subsequent development:

(1) $[P_\lambda,S_{\mu\nu}]_-=0$, $[M_{\kappa\lambda},S_{\mu\nu}]_-=0$. (2.25)

(2) For $m\neq 0$ the eigenmanifold of $\mathbf{P}$ belonging to a given eigenvalue is $(2s+1)$-dimensional.

If $\mathbf{P}'\neq\mathbf{0}$, a basis can be chosen to be eigenvectors of the operator $P^{-1}\mathbf{S}\cdot\mathbf{P}$ (where $P=|\mathbf{P}|$):

$$\frac{\mathbf{S}\cdot\mathbf{P}}{P}|P',\lambda\rangle=\lambda|P',\lambda\rangle \tag{2.26}$$

$$\lambda=-s,\ -s+1,\ \cdots,\ s.$$

λ is called the helicity.

(3) For $m=0$ an eigenmanifold of P is 1-dimensional, and

$$\frac{\mathbf{S}\cdot\mathbf{P}}{P}|P',\lambda\rangle=\lambda|P',\lambda\rangle, \tag{2.27}$$

where $\lambda=\pm s$ for $\Gamma_s^{(\pm)}$.

(4) The vectors $|P',\lambda\rangle$ form a basis of the carrier space.

(5) The operator representing a rotation specified by the Euler angles α,β,γ is given by

$$R(\alpha,\beta,\gamma)=e^{-i\alpha J_z}e^{-i\beta J_y}e^{-i\gamma J_z}, \tag{2.28}$$

where $\mathbf{J}=(J_{23},J_{31},J_{12})$.

(6) $[\mathbf{J},P^{-1}\mathbf{S}\cdot\mathbf{P}]_-=\mathbf{0}$, (2.29)

so

$$[R,P^{-1}\mathbf{S}\cdot\mathbf{P}]_-=0. \tag{2.30}$$

Consequently, if $|\lambda\rangle$ is any eigenvector of $P^{-1}\mathbf{S}\cdot\mathbf{P}$, $P^{-1}\mathbf{S}\cdot\mathbf{P}|\lambda\rangle=\lambda|\lambda\rangle$, then $P^{-1}\mathbf{S}\cdot\mathbf{P}R|\lambda\rangle=\lambda R|\lambda\rangle$.

(7) $e^{-i\pi J_y}P_ze^{i\pi J_y}=-P_z$ (2.31)

(8) In Γ_{ms} and $\Gamma_s^{(\pm)}$

$$e^{2\pi iJ_y}=(-1)^{2s}. \tag{2.32}$$

(9) In any representation the eigenmanifold of $\mathbf{P}$ belonging to eigenvalue $\mathbf{0}$ is invariant under rotations. This manifold therefore generates a unitary representation of the three dimensional rotation group $R(3)$. Such manifolds (for which $\mathbf{P}'=\mathbf{0}$) will be referred to as rest manifolds.

(10) Let Δ_{ms} be the representation of $R(3)$ obtained by restricting Γ_{ms} to $R(3)$ and operating on the rest manifold. Then $\Delta_{ms}=\Delta_s$, where Δ_s is the rep[15] of $R(3)$ belonging to spin s.[16]

III. REDUCTION BY IDEMPOTENTS

One of the most common methods of reducing group representations is the idempotent method,[17] so called because of the use of idempotent operators. Actually there are two idempotent methods, one of which uses characters and the second of which uses matrix elements. The second method will be employed later in this article and will be described briefly here as it applies to $R(3)$.

The invariant group integral will be assumed to be normalized so that the orthogonality relations become

$$\int dR D_{mm'}{}^{(j)}(R)D_{m''m'''}{}^{(k)}(R^{-1})=\frac{8\pi^2}{2j+1}\delta_{jk}\delta_{mm'''}\delta_{m'm''}, \tag{3.1}$$

where $D_{mm}{}^{(j)}(R)$ is the mm'-th matrix element of the matrix representing the rotation R in the $(2j+1)$-dimensional rep Δ_j of $R(3)$.

Let Δ be an arbitrary unitary representation of $R(3)$, and let R denote the unitary operator representing the rotation R in Δ. Then with the aid of the orthogonality relations (3.1) and the invariance of the group integral it can be easily shown that the operators

$$\zeta_{mm'}{}^{(j)}=\frac{2j+1}{8\pi^2}\int dR D_{mm'}{}^{(j)}(R)^*R \tag{3.2}$$

satisfy the relations

$$\zeta_{mm'}{}^{(j)}\zeta_{m''m'''}{}^{(k)}=\delta_{jk}\delta_{m'm''}\zeta_{mm'''}{}^{(j)} \tag{3.3}$$

$$\zeta_{mm'}{}^{(j)\dagger}=\zeta_{m'm}{}^{(j)}. \tag{3.4}$$

From (3.3) one sees that

$$\zeta_{m'm}{}^{(j)}\zeta_{mm}{}^{(j)}=\zeta_{m'm}{}^{(j)} \tag{3.5}$$

$$\zeta_{mm'}{}^{(j)}\zeta_{m'm''}{}^{(j)}=\zeta_{mm''}{}^{(j)} \tag{3.6}$$

$$\zeta_{mm}{}^{(j)2}=\zeta_{mm}{}^{(j)}, \tag{3.7}$$

and from (3.7) one sees that the operators $\zeta_{mm}{}^{(j)}$ are idempotent.

Now let $u_1, u_2, \cdots, u_{2j+1}$ be any set of $2j+1$ vectors in the carrier space of Δ. Again by invariance and orthogonality it can be shown that these vectors form a

other p component; then differentiate keeping the third p constant. Thus, to calculate $M_{01}\psi$ one can express ψ as $\psi(p_0,p_1,p_2)$ or as $\psi(p_0,p_1,p_3)$.

[14] $\gamma_{n\mu}\equiv I\otimes I\otimes\cdots\otimes I\otimes\gamma_\mu\otimes I\otimes\cdots\otimes I$, where γ_μ is a 4×4 Dirac matrix, and is in the nth position.

[15] Γ will denote representations of $\mathfrak{IL}$ and Δ representations of $R(3)$.

[16] For a proof see the Appendix.

[17] Cf. E. P. Wigner, *Group Theory* (Academic Press, Inc., New York, 1959), pp. 113, 114, 118; and J. S. Lomont, *Applications of Finite* Groups (Academic Press, Inc., New York, 1959), p. 75.

basis for the irreducible component Δ_j of Δ, i.e.,

$$Ru_m=\sum_{m'=1}^{2j+1} D_{m'm}^{(j)}(R)u_{m'} \quad (m=1,\cdots,2j+1), \quad (3.8)$$

if and only if

$$\zeta_{m'm}^{(j)}u_{m'}=u_m \quad (m,m'=1,\cdots,2j+1). \quad (3.9)$$

Finally, by using the preceding results one can easily show that if v is any vector in the carrier space of Δ then the set of vectors

$$u_m=\zeta_{mm_0}^{(j)}\, v \ (m_0 \text{ fixed}) \quad (m=1,\cdots,2j+1) \quad (3.10)$$

is a basis for the irreducible component Δ_j of Δ or is a set of zero vectors; i.e., these u_m's satisfy (3.8). The u_m's so constructed will be the zero vector if Δ_j is not a component of Δ.

This completes the description of the idempotent method. However, there is another relation involving the ζ's which will be required later and was in effect derived by Jacob and Wick.[18] The relation is

$$\zeta_{mm'}^{(j)}e^{i\pi J_y}=(-1)^{j-m'}\zeta_{m,-m'}^{(j)}, \quad (3.11)$$

where J_y belongs to the representation Δ of $R(3)$.

The representations of $R(3)$ to which this theory will be applied are infinite-dimensional, but it was shown by Wigner[19] that even infinite-dimensional representations of compact groups can be expressed uniquely as direct sums of finite-dimensional reps.

IV. REDUCTION OF THE LORENTZ GROUP PROBLEM TO A ROTATION GROUP PROBLEM

In this section, product representations of the forms

$$\Gamma_{m_1s_1}\otimes\Gamma_{m_2s_1}, \quad \Gamma_{s_1}^{(\pm)}\otimes\Gamma_{s_2}^{(\pm)}, \quad \text{and} \quad \Gamma_{m_1s_1}\otimes\Gamma_{s_2}^{(\pm)}$$

will be partially reduced. The remaining reduction will involve only the reduction of representations of $R(3)$, and will be performed in the next section by the idempotent method.

The infinitesimal operators of a product representation Γ are

$$P_\lambda=P_\lambda^{(1)}+P_\lambda^{(2)} \quad (4.1)$$

$$J_{\mu\nu}=J_{\mu\nu}^{(1)}+J_{\mu\nu}^{(2)}, \quad (4.2)$$

where the superscripts 1 and 2 label the reps in the product. Consequently, the first Casimir operator is

$$\begin{aligned} C_1&=-P^\lambda P_\lambda \\ &=-P^{(1)\lambda}P_\lambda^{(2)\lambda}P_\lambda^{(2)}-2P^{(1)\lambda}P_\lambda^{(2)} \\ &=C_1^{(1)}+C_1^{(2)}-2P^{(1)\lambda}P_\lambda^{(2)} \\ &=m_1^2+m_2^2-2P^{(1)\lambda}P_\lambda^{(2)}, \end{aligned} \quad (4.3)$$

where either or both m_1 and m_2 may be zero.

[18] See footnote reference 8, p. 417.

[19] E. Wigner, Ann. Math. 40, 149 (1939); see also A. Hurevitsch, Rec. Math. N. S. 13, 79 (1943).

The first question to be answered in this section is: "What are the possible eigenvalues of C_1?" Corresponding to each irreducible component of Γ there will be an eigenvalue m^2 of C_1, and in the rest manifold[20] ($\mathbf{P}'=\mathbf{0}$) of such a component (4.3) and (4.1) become

$$\begin{aligned} C_1&=P_0^2 \\ P^0&=P^{(1)0}+P^{(2)0} \\ &=(\mathbf{P}^{(1)2}+m_1^2)^{\frac{1}{2}}+(\mathbf{P}^{(2)2}+m_2^2)^{\frac{1}{2}}, \end{aligned} \quad (4.4)$$

and since $\mathbf{P}^{(1)}=-\mathbf{P}^{(2)}$ and $P^0=m$,

$$m=(\mathbf{P}^{(1)2}+m_1^2)^{\frac{1}{2}}+(\mathbf{P}^{(1)2}+m_2^2)^{\frac{1}{2}}. \quad (4.5)$$

Since the eigenvalues of $\mathbf{P}^{(i)2}$ vary from 0 to ∞ if $m_i\neq 0$, it follows that, in that case,

$$m_1+m_2\leq m<\infty. \quad (4.6)$$

Since m can assume all values in a continuous range, and since m labels (partially) the irreducible components of Γ, one sees that a direct integral rather than a direct sum should be used in the decomposition of Γ.

The case in which $m_1=0$ (or $m_2=0$) requires special attention because $\mathbf{P}^{(1)\prime}$ (or $\mathbf{P}^{(2)\prime}$) cannot be zero (i.e., have a zero eigenvalue). Thus it would appear that m could not assume the value m_1+m_2. Suppose first that $m_1=m_2=0$. Then there is no manifold in which $\mathbf{P}_1'=\mathbf{P}_2'=\mathbf{0}$, but it is possible for $P_\lambda^{(1)\prime}$ to be a constant times $\mathbf{P}_\lambda^{(2)\prime}$. In that case $m=0$. Second, consider the case $m_1=0$, $m_2\neq 0$. Then in order for m to be m_2 the condition $-m_2^2=P^{\mu\prime}P_\mu'$ must be satisfied, or (dropping primes)

$$\mathbf{P}^{(1)}\cdot\mathbf{P}^{(2)}-|\mathbf{P}^{(1)}|(|P^{(2)}|^2+m_2^2)^{\frac{1}{2}}=0$$

or, letting $\mathbf{P}^{(1)}\cdot\mathbf{P}^{(2)}=|\mathbf{P}^{(1)}||\mathbf{P}^{(2)}|\cos\theta$,

$$\cos\theta=(|P^{(2)}|^2+m_2^2)^{\frac{1}{2}}/|\mathbf{P}^{(2)}|>1.$$

Hence in this case $m\neq m_2$.

The treatment of the exceptional case $m=0$ will be deferred until a later section.

Corresponding to a given nonzero eigenvalue m^2 of C_1, there may be several component reps $\Gamma_{m,J}$ of Γ. Let $\Delta(m)$ be the representation of $R(3)$ obtained by restricting Γ to $R(3)$, and in turn restricting this representation of $R(3)$ to the submanifold of the rest manifold on which $C_1=m^2$. Then according to property (10) of Sec. 2, each component rep $\Gamma_{m,J}$ of Γ when restricted in the foregoing way becomes Δ_J. Thus, by reducing the representation $\Delta(m)$ of $R(3)$, one can find the spin values of the component reps $\Gamma_{m,J}$ together with the multiplicity of each $\Gamma_{m,J}$. The problem is now reduced to the rotation group problem of reducing $\Delta(m)$.

V. SOLUTION OF THE ROTATION GROUP PROBLEM: REDUCTION OF $\Delta(m)$

The representation $\Delta(m)$ of $R(3)$ will be reduced by applying the idempotent method of Sec. 3. The Δ of

[20] There is no rest manifold if $m=0$.

that section is now $\Delta(m)$, and the rotation operator R is now a rotation operator in $\Delta(m)$. To begin with some notation will be needed. Let $|\,|P_z'|,\lambda\rangle$ be a vector in the carrier space of a rep with positive z component of momentum $|P_z'|$, and helicity λ. If the rep has nonzero mass then $|P_z'|=0$ is also allowed. To specify the vector completely its normalization and phase must be given, but here it will be sufficient to assume that one vector has been selected corresponding to each $|P_z'|$, λ-pair. If we let

$$|-|P_z'|,\lambda\rangle=(-1)^{s-\lambda}e^{-i\pi J_y}|\,|P_z'|,\lambda\rangle \tag{5.1}$$

we see from property (7) of Sec. 3 that

$$P_z|-|P_z'|,\lambda\rangle=-|P_z'|\,|-|P_z'|,\lambda\rangle \tag{5.2}$$

and from (2.29) that

$$P^{-1}\mathbf{S}\cdot\mathbf{P}|-|P_z'|,\lambda\rangle=\lambda|-|P_z'|,\lambda\rangle. \tag{5.3}$$

Finally, let

$$|P_z';\lambda_1,\lambda_2\rangle=|\,|P_z'|,\lambda_1\rangle\otimes|-|P_z'|,\lambda_2\rangle, \tag{5.4}$$

where the two vectors whose product is taken lie in the carrier spaces of the two reps whose product is taken. The product vector $|P_z',\lambda_1,\lambda_2\rangle$ is thus in the carrier space of the product representation. Furthermore, it lies in the rest manifold

$$\mathbf{P}|P_z';\lambda_1,\lambda_2\rangle=0. \tag{5.5}$$

The vectors $|P_z';\lambda_1,\lambda_2\rangle$ for which

$$|P_z'|=(2m)^{-1}[(m+m_1+m_2)(m+m_1-m_2)\times(m-m_1+m_2)(m-m_1-m_2)]^{\frac{1}{2}} \tag{5.6}$$

lie in the submanifold belonging to mass m, and will be denoted by

$$|P_z'(m);\lambda_1,\lambda_2\rangle.$$

The idempotent method can now be applied to the reduction of $\Delta(m)$ by defining the vectors

$$|J,M;\lambda_1,\lambda_2\rangle\equiv\zeta_{M,\lambda}{}^{(J)}|P_z'(m);\lambda_1,\lambda_2\rangle, \tag{5.7}$$

where $\lambda=\lambda_1-\lambda_2$, and M can assume the values J, $J-1$, $J-2$, $\cdots$, $-J$. In order for $\zeta_{M,\lambda}{}^{(J)}$ to be defined, it is necessary that

$$|\lambda_1-\lambda_2|\leq J \tag{5.8}$$

and also that

$$J-(s_1+s_2)=\text{integer}. \tag{5.9}$$

Subject to the foregoing restriction (5.9), J can assume any half-integral value from 0 to ∞. Since $|\mathbf{P}^{(1)}|^{-1}\mathbf{S}^{(1)}\cdot\mathbf{P}^{(1)}$ and $|\mathbf{P}^{(2)}|^{-1}\mathbf{S}^{(2)}\cdot\mathbf{P}^{(2)}$ commute with R, they also commute with $\zeta_{M,\lambda}{}^{(J)}$. Hence

$$|\mathbf{P}^{(i)}|^{-1}\mathbf{S}^{(i)}\cdot\mathbf{P}^{(i)}|J,M;\lambda_1,\lambda_2\rangle=\lambda_i|J,M;\lambda_1,\lambda_2\rangle. \tag{5.10}$$

It is now easy to demonstrate the orthogonality of the newly defined vectors, i.e.,

$$\langle J,M;\lambda_1,\lambda_2|J',M';\lambda_1',\lambda_2'\rangle=\delta_{JJ'}\delta_{MM'}\delta_{\lambda_1\lambda_1'}\delta_{\lambda_2\lambda_2'}f(J,\lambda_1,\lambda_2), \tag{5.11}$$

where f is a function of the indicated parameters and the mass. This is derived as follows:

$$\begin{aligned}&\langle J,M;\lambda_1,\lambda_2|J',M';\lambda_1',\lambda_2'\rangle\\&=\langle P_z'(m);\lambda_1,\lambda_2|\zeta_{M,\lambda}{}^{(J)\dagger}\zeta_{M',\lambda'}{}^{(J')}|P_z'(m);\lambda_1',\lambda_2'\rangle\\&=\langle P_z'(m);\lambda_1,\lambda_2|\zeta_{\lambda,M}{}^{(J)}\zeta_{M',\lambda'}{}^{(J')}|P_z'(m);\lambda_1',\lambda_2'\rangle\\&=\delta_{JJ'}\delta_{MM'}\langle P_z'(m);\lambda_1,\lambda_2|\zeta_{\lambda,\lambda'}{}^{(J)}|P_z'(m);\lambda_1',\lambda_2'\rangle.\end{aligned} \tag{5.12}$$

Since $|\mathbf{P}^{(i)}|^{-1}\mathbf{S}^{(i)}\cdot\mathbf{P}^{(i)}$ commutes with $\zeta_{\lambda,\lambda'}{}^{(J)}$ it follows that

$$\begin{aligned}&\langle P_z'(m);\lambda_1,\lambda_2|\zeta_{\lambda,\lambda'}{}^{(J)}|P_z'(m);\lambda_1',\lambda_2'\rangle\\&=\delta_{\lambda_1\lambda_1'}\delta_{\lambda_2\lambda_2'}\langle P_z'(m);\lambda_1,\lambda_2|\zeta_{\lambda\lambda}{}^{(J)}|P_z'(m);\lambda_1,\lambda_2\rangle.\end{aligned} \tag{5.13}$$

Hence

$$\begin{aligned}\langle J,M;\lambda_1,\lambda_2|J',M';\lambda_1',\lambda_2'\rangle&=\delta_{JJ'}\delta_{MM'}\delta_{\lambda_1\lambda_1'}\delta_{\lambda_2\lambda_2'}\\&\times\langle P_z'(m);\lambda_1,\lambda_2|\zeta_{\lambda,\lambda}{}^{(J)}|P_z'(m);\lambda_1,\lambda_2\rangle.\end{aligned} \tag{5.14}$$

Jacob and Wick[8] have shown that for λ and J values subject to the restrictions (5.8) and (5.9),

$$\langle J,M;\lambda_1,\lambda_2|J,M;\lambda_1,\lambda_2\rangle\neq 0. \tag{5.15}$$

Also, they have shown that the vectors $|J,M;\lambda_1,\lambda_2\rangle$ form a complete set in the carrier space of $\Delta(m)$.

Hence, the possible J values are all nonnegative half-integers satisfying (5.9), and the multiplicity of each J value is equal to the number of (λ_1,λ_2)-values satisfying (5.8). Thus, for $J\geq s_1+s_2$ and consistent with (5.9) the multiplicity c_J of J is

$$\begin{aligned}c_J&=(2s_1+1)(2s_2+1)\quad\text{if}\quad m_1\neq 0,\ m_2\neq 0\\&=1\quad\text{if}\quad m_1=m_2=0\\&=2s_1+1\quad\text{if}\quad m_1\neq 0,\ m_2=0.\end{aligned} \tag{5.16}$$

It should be observed that the decomposition of $\Delta(m)$ is independent of m. Some examples are now given:

(1) $s_1=s_2=\frac{1}{2}$, $m_1\neq 0$, $m_2\neq 0$
$\Delta(m)=2\Delta_0+4\Delta_1+4\Delta_2+\cdots$

(2) $s_1=s_2=\frac{1}{2}$, $m_1=m_2=0$, $\lambda_1=\lambda_2=\frac{1}{2}$
$\Delta(m)=\Delta_0+\Delta_1+\Delta_2+\cdots$

(3) $s_1=s_2=\frac{1}{2}$, $m_1=m_2=0$, $\lambda_1=-\lambda_2=\frac{1}{2}$
$\Delta(m)=\Delta_1+\Delta_2+\Delta_3+\cdots$

(4) $s_1=s_2=\frac{1}{2}$, $m_1\neq m_2=0$, $\lambda_2=\pm\frac{1}{2}$
$\Delta(m)=\Delta_0+2\Delta_1+2\Delta_2+\cdots$

(5) $s_1=\frac{1}{2}$, $s_2=1$, $m_1\neq 0$, $m_2\neq 0$
$\Delta(m)=4\Delta_{\frac{1}{2}}+6\Delta_{\frac{3}{2}}+6\Delta_{\frac{5}{2}}+\cdots$.

VI. SYMMETRIZED KRONECKER POWERS

Suppose $V=U\otimes U$ is the Kronecker product of a space U with itself, and let $|v\rangle=|1\rangle\otimes|2\rangle$ be any product vector in V. Then a linear, Hermitian operator P_{12} in

V is defined by the equation

$$P_{12}|v\rangle=|2\rangle\otimes|1\rangle. \tag{6.1}$$

Obviously,

$$P_{12}^2=1, \tag{6.2}$$

so V is the direct sum of the two eigenmanifolds of P_{12} belonging to eigenvalues $+1$ and -1. These are the symmetric and antisymmetric subspaces of V.

Consider now the case in which U is the carrier space of a rep of $\mathcal{GL}$. It is easily seen that P_{12} commutes with the 10 operators P_μ and $K_{\mu\nu}$, and hence that the symmetric and antisymmetric subspaces are invariant under the product representation. Consequently, the symmetric and antisymmetric subspaces generate representations, and these are called the symmetrized and antisymmetrized squares of the rep. Higher symmetrized powers can also be constructed.

The reduction argument for the symmetrized square proceeds as for the ordinary square until the decomposition of the representation $\Delta(m)$ of $R(3)$. Since $\Delta(m)$ is now defined in the symmetric subspace the representation will now be designated by ${}^{(s)}\Delta(m)$. A basis for ${}^{(s)}\Delta(m)$ can be found by simply projecting a basis for $\Delta(m)$ into the symmetric subspace. Such a projection operator is

$$\mathcal{P}=\tfrac{1}{2}(1+P_{12}). \tag{6.3}$$

Thus, to find the effect of $\mathcal{P}$ on a basis vector one need only know the effect of P_{12}. This can be found as follows. If we use (5.7), (5.4), (5.1), (3.11), and property (8) of Sec. 3, we have

$$\begin{aligned}
&P_{12}|J,M;\lambda_1,\lambda_2\rangle\\
&\quad=P_{12}\zeta_{M,\lambda}{}^{(J)}|P_z';\lambda_1,\lambda_2\rangle\\
&\quad=\zeta_{M,\lambda}{}^{(J)}P_{12}|P_z';\lambda_1,\lambda_2\rangle\\
&\quad=\zeta_{M\lambda}{}^{(J)}|-|P_z'(m)|,\lambda_2\rangle\otimes||P_z'(m)|,\lambda_1\rangle\\
&\quad=(-1)^\lambda\zeta_{M,\lambda}{}^{(J)}e^{-iJ_y(1)}e^{i\pi J_y(2)}|P_z'(m);\lambda_2,\lambda_1\rangle\\
&\quad=(-1)^{\lambda-2s}\zeta_{M,\lambda}{}^{(J)}e^{i\pi J_y}|P_z'(m);\lambda_2,\lambda_1\rangle\\
&\quad=(-1)^{J-2s}\zeta_{M,-\lambda}{}^{(J)}|P_z'(m);\lambda_2,\lambda_1\rangle\\
&\quad=(-1)^{J-2s}|J,M;\lambda_2,\lambda_1\rangle,
\end{aligned} \tag{6.4}$$

which is Eq. (46) of Jacob and Wick.[8] Thus

$$\begin{aligned}
|J,M;\lambda_1,\lambda_2\rangle_{(s)}&\equiv\mathcal{P}|J,M;\lambda_1,\lambda_2\rangle\\
&=\tfrac{1}{2}|J,M;\lambda_1,\lambda_2\rangle+(-1)^{J-2s}|J,M;\lambda_2\lambda_1\rangle.
\end{aligned} \tag{6.5}$$

Since J is an integer by (5.9), one has

$$|J,M;\lambda_1,\lambda_2\rangle_{(s)}=(-1)^{J-2s}|J,M;\lambda_{1,-1}\rangle_{(s)}. \tag{6.6}$$

Consequently, if $J-2s$ is odd, $|J,M;\lambda,\lambda\rangle_{(s)}=0$. Thus, the multiplicity c_J of Δ_J for J sufficiently large is

$$\begin{aligned}
c_J&=(s+1)(2s+1) &&\text{if}\quad m\neq0,\ J-2s\text{ even}\\
&=s(2s+1) &&\text{if}\quad m\neq0,\ J-2s\text{ odd}\\
&=1 &&\text{if}\quad m=0,\ J-2s\text{ even}\\
&=0 &&\text{if}\quad m=0,\ J-2s\text{ odd}.
\end{aligned}$$

Examples:

(1) $s=\frac{1}{2}$, $m\neq0$, $2s=1$

${}^{(s)}\Delta(m)=3\Delta_1+\Delta_2+3\Delta_3+\Delta_4+\cdots$

(2) $s=\frac{1}{2}$, $m=0$, $2s=1$

${}^{(s)}\Delta(m)=\Delta_1+\Delta_3+\Delta_5+\cdots$.

VII. $m=0$

The representation of $\mathcal{GL}$ generated by the manifold on which $C_1=0$ will now be reduced. It will be recalled that $m=0$ implies $m_1=m_2=0$.

Since $P_\mu{}^{(1)}$ and $P_\nu{}^{(2)}$ commute, they are simultaneously diagonalizable. Furthermore, on the manifold on which $m=0$ the eigenvalues belonging to a single eigenvector must be related by a proportionality factor

$$P_\mu{}^{(2)\prime}=\alpha P_\mu{}^{(1)\prime}, \tag{7.1}$$

where α is a real, positive constant. Thus, the $m=0$ manifold is spanned by vectors of the form

$$|P_\mu{}^{(1)\prime},\lambda_1\rangle\otimes|\alpha P_\mu{}^{(1)\prime},\lambda_2\rangle. \tag{7.2}$$

Let $\mathfrak{M}_\alpha$ be the manifold spanned by all vectors of the form (7.2) with fixed α, and let

$$\mathcal{O}_\mu{}^{(\alpha)}\equiv P_\mu{}^{(2)}-\alpha P_\mu{}^{(1)}. \tag{7.3}$$

Then $\mathfrak{M}_\alpha$ is the eigenmanifold of $\mathcal{O}_\mu{}^{(\alpha)}$ belonging to eigenvalue zero. Since

$$[\mathcal{O}_\mu{}^{(\alpha)},P_\nu]_-=0 \tag{7.4}$$

$$[\mathcal{O}_\lambda{}^{(\alpha)},J_{\mu\nu}]_-=ig_{\lambda\nu}\mathcal{O}_\mu{}^{(\alpha)}-ig_{\lambda\mu}\mathcal{O}_\nu{}^{(\alpha)}, \tag{7.5}$$

it follows that $\mathfrak{M}_\alpha$ is invariant under $\mathcal{GL}$. Hence $\mathfrak{M}_\alpha$ generates a representation of $\mathcal{GL}$.

It will now be shown that the representation generated by $\mathfrak{M}_\alpha$ is irreducible. It will be shown that an operator A on $\mathfrak{M}_\alpha$ which commutes with the P_μ and $J_{\mu\nu}$ must be a scalar operator. Since P_μ is a complete commuting set in $\mathfrak{M}_\alpha$, $A=A(P)$. If $D(L)$ represents the homogeneous transformation L, then $D^{-1}(L)P^\mu D(L)=L^\mu{}_\nu P^\nu$. Hence,

$$D^{-1}(L)A(P^\mu)D(L)=A(L^\mu{}_\nu P^\nu). \tag{7.6}$$

Since, on the other hand, $D(L)$ commutes with A, it follows that

$$A(L^\mu{}_\nu P^\nu)=A(P^\mu) \tag{7.7}$$

for all values of P_μ in $\mathfrak{M}_\alpha$. Since $P_\mu=(1+\alpha)P_\mu{}^{(1)}$, it follows that

$$A((1+\alpha)L^\mu{}_\nu P^{(1)\nu})=A((1+\alpha)P^{(1)\mu}), \tag{7.8}$$

where $\mathbf{P}^{(1)\prime}$ can assume any real, nonzero value, and $P_0{}^{(1)\prime}=|-\mathbf{P}^{(1)\prime}|$. Thus

$$A(L^\mu{}_\nu P^{(1)\prime\nu})=A(P^{(1)\prime\mu}). \tag{7.9}$$

Hence A is a constant.

The rep generated by $\mathfrak{M}_\alpha$ will now be determined. For

brevity, let $|\psi\rangle = |P^{(1)\prime},\lambda_1\rangle \otimes |\alpha P^{(1)\prime},\lambda_2\rangle$. Then

$$\begin{aligned}
&P^{-1}\mathbf{S}\cdot\mathbf{P}|\psi\rangle \\
&= P^{-1}(\mathbf{S}^{(1)}+\mathbf{S}^{(2)})\cdot(\mathbf{P}^{(1)}+\mathbf{P}^{(2)})|\psi\rangle \\
&= |\,\mathbf{P}^{(1)\prime}+\alpha\mathbf{P}^{(1)\prime}|^{-1}(\mathbf{S}^{(1)}+\mathbf{S}^{(2)})\cdot(\mathbf{P}^{(1)\prime},+\alpha\mathbf{P}^{(1)\prime}|\,|\psi\rangle \\
&= P^{(1)\prime-1}(\mathbf{S}^{(1)}+\mathbf{S}^{(2)})\cdot P^{(1)\prime}|\psi\rangle \\
&= P^{(1)\prime-1}(S^{(1)}\cdot P^{(1)\prime}+\alpha^{-1}S^{(2)}\cdot\alpha P^{(1)\prime}|\,|\psi\rangle \\
&= P^{(1)\prime-1}(S^{(1)}\cdot P^{(1)}+\alpha^{-1}S^{(2)}\cdot P^{(2)})|\psi\rangle \\
&= P^{(1)\prime-1}(\lambda_1 P^{(1)\prime}+\alpha^{-1}\lambda_2\alpha P^{(1)\prime})|\psi\rangle \\
&= (\lambda_1+\lambda_2)|\psi\rangle. \qquad (7.10)
\end{aligned}$$

Hence $\mathfrak{M}_\alpha$ generates the rep

$$\Gamma^{[(\lambda_1+\lambda_2)/(|\lambda_1+\lambda_2|)]}_{|\lambda_1+\lambda_2|}$$

for each α, independent of α.

Since the $m=0$ manifold is the direct sum (or integral) of all $\mathfrak{M}_\alpha$'s, it follows that the representation of $\mathfrak{L}$ generated by the $m=0$ manifold consists of the direct sum (or integral) of an uncountably infinite number of reps

$$\Gamma^{[(\lambda_1+\lambda_2)/(|\lambda_1+\lambda_2|)]}_{|\lambda_1+\lambda_2|}$$

with one for each real positive number α.

The case $m=0$ arises in the products $\Gamma_{s_1}{}^{(\pm)}\otimes\Gamma_{s_2}{}^{(\pm)}$, but it also arises in the symmetrized products $\Gamma_s{}^{(\pm)}\mathbin{\mathbb{A}}\Gamma_s{}^{(\pm)}$. The $m=0$ manifold arising in the $\Gamma_s{}^{(\pm)}\mathbin{\mathbb{A}}\Gamma_s{}^{(\pm)}$ problem is just the symmetric subspace of the $m=0$ manifold in the $\Gamma_s{}^{(\pm)}\otimes\Gamma_s{}^{(\pm)}$ problem. The manifolds $\mathfrak{M}_\alpha$, however, are neither symmetric nor antisymmetric. Let $\mathfrak{N}_\alpha$ be the manifold spanned by vectors of the form

$$|\alpha P_\mu{}^{(2)\prime},\lambda_1\rangle\otimes|P^{(2)\prime},\lambda_2\rangle.$$

$\mathfrak{N}_\alpha$ is invariant and generates

$$\Gamma^{[(\lambda_1+\lambda_2)/(|\lambda_1+\lambda_2|)]}_{|\lambda_1+\lambda_2|}.$$

The manifold $M_\alpha=\mathfrak{M}_\alpha\oplus\mathfrak{N}_\alpha$ is easily seen to be invariant under P_{12}. The symmetric and antisymmetric subspaces of M_α again generate

$$\Gamma^{[(\lambda_1+\lambda_2)/(|\lambda_1+\lambda_2|)]}_{|\lambda_1+\lambda_2|}.$$

Hence "half" of the component reps of the $m=0$ component of $\Gamma_s{}^{(\pm)}\otimes\Gamma_s{}^{(\pm)}$ belong to the $m=0$ component of $\Gamma_s{}^{(\pm)}\mathbin{\mathbb{A}}\Gamma_s{}^{(\pm)}$.

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APPENDIX

It will be shown here that the group of rotation operators belonging to $\Gamma_{m,s}$ yields the representation Δ_s of $R(3)$ when applied to the rest manifold.

First the case $s=\frac{1}{2}$ will be treated. The vectors in the rest manifold satisfy

$$\mathbf{P}\psi(p)=\mathbf{0}, \qquad (A\text{-}1)$$

and since $\mathbf{P}\psi(p)=\mathbf{p}\psi(p)$, it follows that

$$\mathbf{p}\psi(p)=0. \qquad (A\text{-}2)$$

Hence

$$\psi(p)=\phi\delta^{(3)}(\mathbf{p}), \qquad (A\text{-}3)$$

where ϕ is independent of $\mathbf{p}$. The wave equation (2.14) applied to the $\psi(p)$ of (A-3) becomes

$$\beta\phi=\phi. \qquad (A\text{-}4)$$

There are two linearly independent solutions of (A-4), and since $[S_z,\beta]=0$, they can be chosen to be eigenvectors of S_z. They are the spin up and spin down solution $\phi_\pm$. By applying S_x and S_y to $\phi_\pm$ one finds that they generate $\Delta_{\frac{1}{2}}$. Since $\delta^{(3)}(\mathbf{p})$ is invariant under a rotation the rest manifold of $\Gamma_{m,\frac{1}{2}}$ generates $\Delta_{\frac{1}{2}}$.

For higher spins ($s>\frac{1}{2}$) Eq. (A-3) is still valid. A set of basis ϕ's is now

$$\begin{aligned}
\phi_{++\cdots++} &= \phi_+\otimes\phi_+\otimes\cdots\otimes\phi_+\otimes\phi_+ \\
\phi_{++\cdots+-} &= \sum_P P\phi_+\otimes\phi_+\otimes\cdots\otimes\phi_+\otimes\phi_- \qquad (A\text{-}5)\\
&\vdots \\
\phi_{--\cdots--} &= \phi_-\otimes\phi_-\otimes\cdots\otimes\phi_-\otimes\phi_-,
\end{aligned}$$

where P permutes the suffixes, and the sum is over all permutations. The number of basis vectors is $2s+1$, and the representation of $\mathbf{S}$ generated by them is the $2s$th symmetrized Kronecker power of $\Delta_{\frac{1}{2}}$. Since this is Δ_s the desired result is established.

New Theorem in the Classical Ensemble Theory

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In the framework of the classical ensemble theory a theorem is proved which is sufficient to justify the classical statistical mechanics.

Our result can be stated as follows. Let us consider a fixed and otherwise arbitrary subdivision in cells I_ν ($\nu=1, 2, \cdots, N$) of the energy shell I of an isolated dynamical system: Having introduced a suitable definition of functional average, we prove that for "almost all" the initial Liouville density functions $\rho(p',q';0)$ we have

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\left\{\left[\int_{I_\nu}\rho(p',q';t)dp'dq'-\frac{\sigma_\nu}{\sigma}\right]^2\right\}=0,$$

where σ_ν and σ are the measures of I_ν and I, respectively. The unitarity of the Koopman-von Neumann time-evolution operator is the only dynamical property needed to establish this theorem. On the basis of our result, it can be shown that systems with very many degrees of freedom satisfy the laws of statistical mechanics.

I.

THE justification of the classical statistical mechanics is usually based, in the ensemble theory approach, on the second mixing theorem of Hopf.[1] This theorem can be stated as follows: If (and only if) the dynamical system is metrically transitive in the direct sum space $\Sigma=\Gamma\oplus\Gamma$ (where Γ is the phase-space of the system) we have

$$M\left\{\left[\int_{I_\nu}\rho(C,t)dp'dq'-\frac{\sigma_\nu}{\sigma}\right]^2\right\}=0, \tag{1}$$

where M denotes time averaging

$$\lim_{T\to\infty}(1/T)\int_0^T dt(\cdots),$$

$\rho(C,t)$ is any positive definite function of the points $C\equiv(p',q')$ of Γ, I_ν is any region of the energy shell I, σ_ν and σ are the measures of I_ν and I, respectively, i.e., $\int_{I_\nu}dp'dq'=\sigma_\nu$; $\int_I dp'dq'=\sigma$. In other words, this ergodic theorem states that for any $\rho(C,0)$ the time evolution is such that $\rho(C,t)$ is nearly always practically uniform in the energy shell.

As it is well known, it has not yet been possible to ascertain which dynamical systems are metrically transitive. In order to avoid this difficulty we have reexamined the problem and we have given a theorem, the validity of which does not depend on any ergodicity condition like metric transitivity. This theorem is sufficient to justify statistical mechanics. It can be considered, from a methodological point of view, on the one hand as the classical analog of a quantum theorem recently given,[2] and on the other hand, as the counterpart in the ensemble theory of the theorem of Khinchin, Truesdell and Morgenstern.[3]

II.

The Koopman-von Neumann's formulation of classical dynamics in Hilbert space[4] is the proper tool for dealing with our problem. Since this formulation is not generally known to physicists, we have briefly sketched it in the Appendix.

Let $\rho(p',q';t)$ be the Liouville function of any statistical ensemble representing an isolated system with given energy. If we put with a notation *à la* Dirac:

$$|\rho(t)\rangle=\int_I\rho(p',q';t)|p'\rangle|q'\rangle dp'dq', \tag{2}$$

the equation of motion in the classical Schroedinger picture can be written

$$|\rho(t)\rangle=U(t,0)|\rho(0)\rangle, \tag{3}$$

where $U(t,0)$ denotes the (unitary) time-evolution operator.

Let us now consider an arbitrary subdivision of the energy shell I in phase-cells I_ν ($\nu=1, 2, \cdots, N$) and let us call $\varphi_\nu(p',q')$ the characteristic function of the νth cell, i.e., the function which is equal to one when

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[1] E. Hopf, *Ergodentheorie* (Springer-Verlag, Berlin, Germany, 1937), p. 37.

[2] P. Bocchieri and A. Loinger, Phys. Rev. **114**, 948 (1959); G. M. Prosperi and A. Scotti, Nuovo cimento **13**, 1007 (1959).

[3] A. I. Khinchin, *Mathematical Foundations of Statistical Mechanics* (Dover Publications, New York, 1949), Sec. 13; C. Truesdell and D. Morgenstern, Ergeb. exak. Naturw. **13**, 286 (1958).

[4] B. O. Koopman, Proc. Natl. Acad. Sci. U. S. **17**, 315 (1931); J. von Neumann, Ann. Math. **33**, 587 (1932).

the point (p',q') belongs to I_ν and to zero otherwise. The corresponding vector $|\varphi_\nu\rangle$ (which we will call the characteristic vector of I_ν) is the standard ket of the orthogonal basis $|p'\rangle|q'\rangle \equiv |p',q'\rangle$ whose labels p', q' belong to I_ν. We have

$$\langle\varphi_\nu|\varphi_\nu\rangle = \int_I \varphi_\nu^2(p',q')dp'dq' = \sigma_\nu; \tag{4}$$

$$\langle\varphi_\mu|\varphi_\nu\rangle = 0; \quad (\mu \neq \nu). \tag{5}$$

Consequently, the probability $P_\nu(t)$ of finding a system of the ensemble in the cell I_ν at time t can be written

$$P_\nu(t) = \int_{I_\nu} \rho(p',q';t)dp'dq' = \langle\varphi_\nu|\rho(t)\rangle = \langle\varphi_\nu|U(t,0)|\rho(0)\rangle. \tag{6}$$

Let us now call $\mathfrak{B}$ an averaging operation on the initial kets $|\rho(0)\rangle$ which gives the same weight to all the possible $|\rho(0)\rangle$'s. If M denotes time averaging, we shall have

$$\mathfrak{B}MP_\nu(t) = \mathfrak{B}M\langle\varphi_\nu|U(t,0)|\rho(0)\rangle = \{M\langle\varphi_\nu(t)|\}\{\mathfrak{B}|\rho(0)\rangle\}, \tag{7}$$

where $\langle\varphi_\nu(t)| = \langle\varphi_\nu|U(t,0)$. The averaging $\mathfrak{B}$ must be performed taking into account the following subsidiary condition [normalization of the function $\rho(p',q';t)$]:

$$\langle\varphi|\rho(0)\rangle = 1, \tag{8}$$

where $\langle\varphi|$ is the characteristic bra of the energy shell

$$\langle\varphi| = \sum_1^N{}_\nu \langle\varphi_\nu|; \quad \langle\varphi|\varphi\rangle = \sigma. \tag{9}$$

In order to perform the operation $\mathfrak{B}$, we shall subdivide all the possible $|\rho(0)\rangle$'s in classes in such a way that every class contains the $|\rho(0)\rangle$'s having the same Hilbert norm, and we shall perform first the averaging within every class. Let us consider a certain class C'. Since the vectors $|\rho(0)\rangle$ belonging to C' form the "lateral surface" of the "rotation cone" the axis of which has the same direction as $|\varphi\rangle$, we have, if $\mathfrak{B}'$ denotes the averaging within C':

$$\mathfrak{B}'|\rho(0)\rangle = a'|\varphi\rangle, \tag{10}$$

where a' is a number; but a' does not depend on the chosen class: in fact, averaging relation (8) we obtain

$$\mathfrak{B}'\langle\varphi|\rho(0)\rangle = \langle\varphi|\mathfrak{B}'|\rho(0)\rangle = a'\langle\varphi|\varphi\rangle = 1;$$

from which,

$$a' = 1/\sigma; \tag{11}$$

and therefore:

$$\mathfrak{B}'|\rho(0)\rangle = (1/\sigma)|\varphi\rangle, \tag{10'}$$

$$\mathfrak{B}|\rho(0)\rangle = (1/\sigma)|\varphi\rangle. \tag{12}$$

By substituting into Eq. (7) we finally obtain

$$\mathfrak{B}MP_\nu(t) = \{M\langle\varphi_\nu(t)\}\{\mathfrak{B}|\rho(0)\rangle\} = \{M\langle\varphi_\nu(t)|\}(1/\sigma)|\varphi\rangle = (1/\sigma)\{M\langle\varphi_\nu|U(t,0)\}|\varphi\rangle = 1/\sigma\langle\varphi_\nu|\varphi\rangle = \sigma_\nu/\sigma, \tag{13}$$

where use has been made of the evident relation $U(t,0)|\varphi\rangle = |\varphi\rangle$.

We notice that result (13) has been reached by using only the linearity and symmetry properties of the operation $\mathfrak{B}$. The last property is the natural generalization of that symmetry property, which, as it will be apparent later, is an obvious consequence of the equiprobability of all the possible $|\rho(0)\rangle$'s.

III.

It is now necessary, in view of further developments, to give a more precise definition of the operation $\mathfrak{B}$, of which we have employed till now only some formal properties.

To this end, let us subdivide every cell I_ν into $k\sigma_\nu$ subcells $I_{\nu j}$ ($\nu = 1, 2, \cdots, N$; $j = 1, 2, \cdots, k\sigma_\nu$) of *equal* measure. Consequently, the energy shell I will be subdivided into

$$k\sigma = k\sum_1^N{}_\nu \sigma_\nu$$

subcells each of measure $1/k$. If we put $\rho(p',q';0) \equiv c(p',q')$, we will then obtain

$$|\rho(0)\rangle = \sum_1^N{}_\nu \int_{I_\nu} c(p',q')|p',q'\rangle dp'dq' = \sum_1^N{}_\nu \sum_1^{k\sigma_\nu}{}_j \int_{I_{\nu j}} c(p',q')|p',q'\rangle dp'dq'. \tag{14}$$

We shall now have approximately

$$|\rho(0)\rangle \simeq \sum_1^N{}_\nu \sum_1^{k\sigma_\nu}{}_j c_{\nu j} \int_{I_{\nu j}} |p',q'\rangle dp'dq' = \sum_1^N{}_\nu \sum_1^{k\sigma_\nu}{}_j c_{\nu j}|\varphi_{\nu j}\rangle, \tag{15}$$

where the $|\varphi_{\nu j}\rangle$ are the characteristic vectors of the subcells $I_{\nu j}$ and $c_{\nu j}$ is the average of $c(p',q')$ within $I_{\nu j}$. The approximation made becomes obviously better and better as the number of the subcells $I_{\nu j}$ increases, i.e., as the number k gets larger and larger. We obtain

$$MP_\nu(t) = M\langle\varphi_\nu|\rho(t)\rangle = M\langle\varphi_\nu(t)|\rho(0)\rangle \simeq M\sum_1^N{}_{\nu'} \sum_1^{k\sigma_{\nu'}}{}_{j'} c_{\nu' j'}\langle\varphi_\nu(t)|\varphi_{\nu' j'}\rangle = \sum_1^N{}_{\nu'} \sum_1^{k\sigma_{\nu'}}{}_{j'} c_{\nu' j'} M\langle\varphi_\nu(t)|\varphi_{\nu' j'}\rangle. \tag{16}$$

Since the vectors $|\rho(0)\rangle$ are now, in this approximation, vectors of a space with a finite number $k\sigma$ of dimensions, the operation $\mathfrak{B}$ (which, to denote the approximation made, will be called $\mathfrak{B}_k$) is an averaging on the components $c_{\nu j}$, perfectly defined by the condition that all the possible $|\rho(0)\rangle$'s have the same weight. From Eq. (8) we obtain immediately the subsidiary condition to be satisfied by the components $c_{\nu j}$:

$$1=\langle\varphi|\rho(0)\rangle=\sum_{1}^{N}{}_{\nu,\nu'}\sum_{1}^{k\sigma_{\nu'}}{}_{j'}\langle\varphi_\nu|\varphi_{\nu'j'}\rangle c_{\nu'j'}$$
$$=\frac{1}{k}\sum_{1}^{N}{}_{\nu}\sum_{1}^{k\sigma_\nu}{}_{j}c_{\nu j}. \quad (17)$$

$\mathfrak{B}_k$-averaging formula (16) under condition (17), we obtain

$$\mathfrak{B}_k M\mathrm{P}_\nu(t)=\sum_{1}^{N}{}_{\nu'}\sum_{1}^{k\sigma_{\nu'}}{}_{j'}\mathfrak{B}_k(c_{\nu'j'})M\langle\varphi_\nu(t)|\varphi_{\nu'j'}\rangle, \quad (18)$$

from which result (13) follows immediately, for every value of k.

Therefore, we may conclude this section remarking that the prescription

$$\mathfrak{B}(\cdots)\equiv\lim_{k\to\infty}[\mathfrak{B}_k(\cdots)_k]$$

represents a physically reasonable and mathematically precise definition of the functional averaging in question. We notice, however, that this procedure does not allow one to conclude straightforwardly that a measure in the functional space is associated with the averaging defined in this way. *A priori* a certain amount of caution is suggested by the well-known fact that the limit of a measure is not necessarily a measure.[5] This point will be the object of further investigation.

IV.

We are going now to prove a relation of the following kind:

$$\mathfrak{B}M\{[\mathrm{P}_\nu(t)-(\sigma_\nu/\sigma)]^2\}\ll\sigma_\nu^2/\sigma^2.$$

Taking into account result (13), one has to prove that

$$\mathfrak{B}M\mathrm{P}_\nu^2(t)-(\sigma_\nu^2/\sigma^2)\ll\sigma_\nu^2/\sigma^2. \quad (19)$$

But

$$\mathfrak{B}M\mathrm{P}_\nu^2(t)=\mathfrak{B}M\{\langle\varphi_\nu(t)|\rho(0)\rangle\langle\varphi_\nu(t)|\rho(0)\rangle\}$$
$$\simeq\sum_{1}^{N}{}_{\mu,\mu'}\sum_{1}^{k\sigma_\mu,k\sigma_{\mu'}}{}_{j,j'}\mathfrak{B}_k(c_{\mu j}c_{\mu'j'})$$
$$\cdot M\{\langle\varphi_\nu(t)|\varphi_{\mu j}\rangle\langle\varphi_\nu(t)|\varphi_{\mu'j'}\rangle\}, \quad (20)$$

from which it follows, first of all, that $\mathfrak{B}$ and M commute. For sake of convenience we shall now replace the indices (μ,j) by the unique index $i=1, 2, \cdots, k\sigma$. We have then to evaluate the average

$$\mathfrak{B}_k(c_ic_{i'}) \quad (21)$$

under the subsidiary condition:

$$\sum_{1}^{n}{}_{i}c_i=k; \quad (n\equiv k\sigma). \quad (22)$$

Consider, in the real n-dimensional Euclidean space, the hypertetrahedron having vertices in the origin of the reference frame $0c_1c_2\cdots c_n$ and in the points in which the plane (22) intersects the axes of this frame. If T is the hypertriangle common to the hypertetrahedron and to the plane (22), we have evidently

$$\mathfrak{B}_k(c_ic_{i'})\overset{\text{Def}}{=}\left(\int_T c_ic_{i'}dT\Big/\int_T dT\right), \quad (23)$$

where dT is the Euclidean measure of the surface element of T. Manifestly,

$$\int_T dT=\frac{(\text{Volume of the hypertetrahedron})\cdot n}{\text{Height of the hypertetrahedron}}$$
$$=\frac{(k^n/n!)n}{\underbrace{[(k/n)^2+\cdots(k/n)^2]^{\frac{1}{2}}}_{n}}=\frac{k^{n-1}n^{\frac{1}{2}}}{(n-1)!}. \quad (24)$$

It is clearly sufficient to evaluate the two typical averages $\mathfrak{B}_k(c_1^2)$ and $\mathfrak{B}_k(c_1c_2)$. We have

$$\mathfrak{B}_k(c_1^2)=\left[\frac{k^{n-1}n^{\frac{1}{2}}}{(n-1)!}\right]^{-1}\int_T c_1^2dT=\frac{(n-1)!}{k^{n-1}n^{\frac{1}{2}}}\frac{1}{\cos(|\varphi\rangle,c_n)}$$
$$\times\int_{T'}c_1^2dT'=\frac{(n-1)!}{k^{n-1}}\int_{T'}c_1^2dT',$$

where

$$\int_{T'}dT'=\int_0^k dc_1\int_0^{k-c_1}dc_2\cdots\int_0^{k-c_1-c_2-\cdots-c_{n-2}}dc_{n-1}$$
$$=\frac{k^{n-1}}{(n-1)!}; \quad [\cos(|\varphi\rangle,c_n)=n^{-\frac{1}{2}}]$$

is the measure of the hypertriangle orthogonal projection of T on the plane $c_n=0$. But

$$\int_{T'}c_1^2dT'=\int_0^k c_1^2dc_1\int_0^{k-c_1}dc_2\cdots\int_0^{k-c_1-\cdots-c_{n-2}}dc_{n-1}$$
$$=\int_0^k c_1^2\frac{(k-c_1)^{n-2}}{(n-2)!}dc_1;$$

[5] P. Lévy, *Problèmes Concrets d'Analyse Fonctionelle* (Gauthier-Villars Paris, France, 1951), p. 293.

and consequently

$$\mathfrak{B}(c_1^2)=\frac{n-1}{k^{n-1}}\int_0^k c_1^2(k-c_1)^{n-2}dc_1=\frac{2k^2}{n(n+1)}. \quad (25)$$

Similarly, we find

$$\mathfrak{B}(c_1c_2)=k^2/n(n+1). \quad (26)$$

Substituting in Eq. (20) one obtains

$$\begin{aligned}\mathfrak{B}M\mathrm{P}_\nu^2(t)\simeq&\sum_1^N{}_\mu\sum_1^{k\sigma_\mu}{}_j\frac{2k^2}{n(n+1)}\\&\cdot M\{[\langle\varphi_\nu(t)\,|\,\varphi_{\mu j}\rangle]^2\}+\sum_1^N{}_\mu\sum_1^{k\sigma_\mu}{}_{j\neq j'}\frac{k^2}{n(n+1)}\\&\cdot M\{\langle\varphi_\nu(t)\,|\,\varphi_{\mu j}\rangle\langle\varphi_\nu(t)\,|\,\varphi_{\mu j'}\rangle\}\\&+\sum_1^N{}_{\mu\neq\mu'}\sum_1^{k\sigma_\mu,k\sigma_{\mu'}}{}_{j,j'}\frac{k^2}{n(n+1)}\\&\cdot M\{\langle\varphi_\nu(t)\,|\,\varphi_{\mu j}\rangle\langle\varphi_\nu(t)\,|\,\varphi_{\mu' j'}\rangle\}\\=&\sum_1^N{}_\mu\sum_1^{k\sigma_\mu}{}_j\frac{k^2}{n(n+1)}\\&\cdot M\{[\langle\varphi_\nu(t)\,|\,\varphi_{\mu j}\rangle]^2\}+\sum_1^N{}_{\mu,\mu'}\sum_1^{k\sigma_\mu,k\sigma_{\mu'}}{}_{j,j'}\frac{k^2}{n(n+1)}\\&\cdot M\{\langle\varphi_\nu(t)\,|\,\varphi_{\mu j}\rangle\langle\varphi_\nu(t)\,|\,\varphi_{\mu' j'}\rangle\}\\=&\frac{k^2}{n(n+1)}\left(\frac{\sigma_\nu}{k}+\sigma_\nu^2\right)\\=&\frac{\sigma_\nu(\sigma_\nu+1/k)}{\sigma(\sigma+1/k)}\xrightarrow[(k\to\infty)]{}\frac{\sigma_\nu^2}{\sigma^2}. \quad (27)\end{aligned}$$

We obtain, in conclusion,

$$\mathfrak{B}M\mathrm{P}_\nu^2(t)-(\sigma_\nu^2/\sigma^2)=0, \quad (28)$$

from which it follows immediately

$$\mathfrak{B}M\left\{\left[\sum_1^N{}_\nu\,\mathrm{P}_\nu(t)-\frac{\sigma_\nu}{\sigma}\right]^2\right\}=0. \quad (29)$$

Equation (29) asserts that *for any subdivision in cells* I_ν $(\nu=1, 2, \cdots, N)$ *of the energy shell* I, *relations*

$$\mathrm{P}_\nu(t)=\sigma_\nu/\sigma;\quad(\nu=1, 2, \cdots, N) \quad (30)$$

are satisfied at the overwhelming majority of the time instants t *for "almost all" the initial vectors* $|\rho(0)\rangle$. Obviously, the set of the exceptional initial vectors for which relations (30) do not hold true depends both on the subdivision in cells and on the instant t.

Result (30) is valid independently of the value of the number g of degrees of freedom. In this respect it differs from its quantum analogue, which is only asymptotically valid for large values of g. This is a consequence of the fact that the structure of the "concrete" functional space employed in this paper is different from that of the space of quantum theory.

The only assumption essential to the validity of Eqs. (30) is the unitarity of the Koopman-von Neumann time evolution operator, i.e., the canonicity of the equations of motion. However, in order to justify statistical mechanics on the basis of Eqs. (30)—first of all in order to deduce the canonical distribution law—the assumption that g is a very great number is needed, as one can see easily bearing in mind a well-known procedure.[6]

In conclusion, it has been possible to get rid of any hypothesis of metric transitivity by giving up the purpose of establishing an ergodic theorem valid for all the initial Liouville functions $\rho(0)$. The result so obtained, except for the necessary assumption of unitarity of the evolution operator, depends only on the geometrical structure of the considered functional space.

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APPENDIX

Koopman-von Neumann's Formulation of Classical Mechanics in Hilbert Space

(i) Let $\mathfrak{R}$ be the Hilbert space of the Lebesgue-measurable and square integrable functions of the points of the $2g$-dimensional phase-space Γ and let $\mathfrak{R}_D$ be its extension in the sense of Dirac.

Let us consider in $\mathfrak{R}_D$ a representation characterized by the eigenkets $|p_j'\rangle$ and $|q_j'\rangle$ corresponding to the numerical values p_j' and q_j' of the dynamical variables p_j and q_j $(j=1, 2, \cdots, g)$. The standard ket $\rangle$ of this representation will obviously be given by the relation

$$\rangle=\int\int|p',q'\rangle dp'dq', \quad (1A)$$

where

$$|p',q'\rangle\equiv|p'\rangle|q'\rangle;$$
$$dp'dq'\equiv dp_1'dp_2'\cdots dp_g'dq_1'dq_2'\cdots dq_g'.$$

The abstract vector corresponding to any dynamical variable $f(p,q)$ can be written as follows:

$$f(p,q)\rangle=\int\int f(p',q')\,|\,p',q'\rangle dp'dq'\equiv|\,f\rangle.$$

Let $(p,q)\to(P,Q)$ be any canonical transformation and $F(p,q)$ a function such that $F(P,Q)\equiv f(p,q)$. Then the

[6] See e.g. the book of Khinchin quoted in footnote reference 3, p. 91.

Hilbert transformation U defined by the relation

$$F(p,q)\rangle\equiv|F\rangle=U|f\rangle \tag{2A}$$

is unitary, as follows immediately from the fact that the Jacobian of a canonical transformation is equal to ± 1. If we perform a second canonical transformation $(P,Q)\rightarrow(\pi,\chi)$, we shall have $|\psi\rangle=V|F\rangle=VU|f\rangle$, from which it can be concluded that the canonical transformation group induces a group of unitary transformations in $\mathfrak{R}_D$. One gets easily convinced that the algebraic relations and the reality properties are invariant under the group of the U transformations.

To an infinitesimal canonical transformation characterized by a parameter ϵ and a generating function $G(p,q)$:

$$\delta f(p,q)=\epsilon\{G(p,q),f(p,q)\}=i\epsilon\mathfrak{D}[G(p,q)]f(p,q), \tag{3A}$$

where

$$\mathfrak{D}[G(p,q)]\equiv\frac{1}{i}\sum_{1}^{s}{}_j\left(\frac{\partial G}{\partial q_j}\frac{\partial}{\partial p_j}-\frac{\partial G}{\partial p_j}\frac{\partial}{\partial q_j}\right), \tag{4A}$$

it will correspond a unitary transformation

$$\delta|f\rangle=i\epsilon\hat{G}|f\rangle, \tag{5A}$$

where $\hat{G}$ is an Hermitean operator which coincides with $\mathfrak{D}[G]$, as it can be easily seen.

(ii) Let us consider an isolated dynamical system the Hamiltonian of which is $H(p,q)$. The generating operator of the unitary transformation induced by an infinitesimal time displacement $t\rightarrow t+\delta t$ is the Hermitean operator $\hat{H}$. Let

$$\hat{H}=\int_{-\infty}^{+\infty}\lambda dE_\lambda \tag{6A}$$

be its spectral decomposition, in the customary von Neumann notation. If $U^*(t,0)$ (*≡Hermitean conjugate) is the time evolution operator of the vectors $|f\rangle$:

$$|f(t)\rangle=U^*(t,0)|f(0)\rangle, \tag{7A}$$

we shall have

$$U^*(t,0)=\exp(i\hat{H}t)=\int_{-\infty}^{+\infty}\exp(i\lambda t)dE_\lambda. \tag{8A}$$

To find the spectral decomposition of $\hat{H}$ is equivalent to solve the canonical equations of motion. In fact, the equations

$$p(t)\rangle=\int_{-\infty}^{+\infty}\exp(i\lambda t)dE_\lambda p(0)\rangle; \tag{9A}$$

$$q(t)\rangle=\int_{-\infty}^{+\infty}\exp(i\lambda t)dE_\lambda q(0)\rangle \tag{10A}$$

are evidently equivalent to the Fourier expansions of the solutions of the Hamilton equations.

(iii) The considerations developed in (ii) make reference to a (classical) Heisenberg picture. But it is also possible to keep the dynamical variables fixed and let the Liouville ket develop in time, obtaining in this way a Schroedinger picture. (Obviously, in the pure case the Liouville function will actually be a δ function of Dirac.)[7] The equation of motion of the Liouville ket $|\rho(t)\rangle$ is

$$|\rho(t)\rangle=U(t,0)|\rho(0)\rangle. \tag{11A}$$

(iv) Finally, we remember that also quantum theory can be developed according to a scheme analogous to the one sketched here for the classical theory. To this end, it is sufficient to consider a Hilbert space whose elements $|\alpha\rangle$, $|\beta\rangle$, $\cdots$ are the operators α, β, $\cdots$ of the conventional formulation, to give a suitable definition of scalar product (one puts $\langle\alpha|\beta\rangle=\text{Trace }(\alpha^*\beta)$), etc.[8]

[7] The possibility of considering different pictures in classical dynamics has been emphasized by U. Uhlhorn, Arkiv Fysik **11**, 87 (1956).

[8] See J. von Neumann, Ann. Math. **41**, 94 (1940).