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Multiple Density Correlations in a Many-Particle System*†

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A closed expression similar to the Ursell-Mayer expansion is obtained for the static multiple density correlation function $I_n = \langle \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_n} \rangle$ of a many-particle system. It is shown that I_n breaks into products of lower ones, if there exist partial momentum conservations among the \mathbf{k} 's. Using the convolution approximation for the n -particle correlation function, we evaluate I_n in a closed form. The result is shown to be accurate in the small k region.

I. INTRODUCTION

The static multiple density correlation functions

$$I_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) = \langle \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_n} \rangle \tag{1}$$

play an important role in the study of many-particle systems. The notation $\langle \rangle$ denotes the expectation value for a quantum mechanical system or the canonical ensemble average for a classical system; $\rho_{\mathbf{k}}$ is the density fluctuation. In the theory of quantum liquids,¹ for example, I_n 's are the overlapping matrix elements of the phonon states. A detailed knowledge of these integrals would then permit the construction of a complete set of orthonormal states. In the configurational space we have

$$\rho_{\mathbf{k}} = \sum_{i=1}^N \exp(i\mathbf{k} \cdot \mathbf{r}_i), \tag{2}$$

where \mathbf{r}_i is the coordinate of the i th particle and N the total number of particles. The evaluation of I_n then requires a knowledge of the n -particle distribution function g_n . In order to have a reasonable estimate of these matrix elements, one usually uses the Kirkwood superposition approximation² or the convolution approximation^{3,4} for g_n . It is quite difficult, however, to assess the accuracy of these estimates. Furthermore, the algebra involved in these evaluations is quite tedious. For example, one has to consider explicitly whether there exist partial momentum conservations among the \mathbf{k} 's. Besides a few special cases that have been considered,⁵⁻⁹ no general expression is known for I_n .

In this paper we shall consider this general problem. We first derive in Sec. II a general expression for I_n . From this expression and the assumed cluster property of the distribution functions, we are able to see that I_n breaks into product of lower ones if there exist partial momentum conservations among the \mathbf{k} 's. Consequently, some of the results previously obtained using the superposition approximation are seen to be exact. This general discussion also permits us to assess the accuracy of the estimation obtained by using the convolution approximation. In Sec. III we use the convolution approximation to evaluate I_n . A closed expression is obtained and is shown to be accurate in the small k region. Some applications of our result are given in Sec. IV.

II. GENERAL FORMULATION

The quantity of interest is I_n defined by Eq. (1). Explicitly we write

$$I_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) = Q_N^{-1} \int W_n \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_n} \cdot d\mathbf{r}_1 \cdots d\mathbf{r}_N, \tag{3}$$

where

$$Q_N = \int W_N d\mathbf{r}_1 \cdots d\mathbf{r}_N$$

and W_N is symmetric in the particle coordinates $\{\mathbf{r}_1, \cdots, \mathbf{r}_N\}$ and is given by

$$W_N = \exp[-V(\mathbf{r}_1, \cdots, \mathbf{r}_N)/kT] \tag{4a}$$

for a classical system,

$$W_N = |\psi(\mathbf{r}_1, \dots, \mathbf{r}_N)|^2 \tag{4b}$$

for a quantum mechanical system.

Here V is the total potential energy and ψ is the wavefunction describing the system.

Let us define as in Ref. 4 the n -particle distribution function

$$g_n(\mathbf{r}_1, \dots, \mathbf{r}_n) = \frac{N!}{(N-n)!} Q_N^{-1} \rho^{-n} \times \int W_N d\mathbf{r}_{n+1} \dots d\mathbf{r}_N, \tag{5}$$

where ρ is the particle number density. An immediate consequence of this definition is the sequential relation

$$\rho \int g_{n+1}(\mathbf{r}_1, \dots, \mathbf{r}_{n+1}) d\mathbf{r}_{n+1} = (N-n)g_n(\mathbf{r}_1, \dots, \mathbf{r}_n). \tag{6}$$

The following cluster condition is also expected to hold for an infinite homogeneous and isotropic system such as a liquid:

$$\lim_{r_i \rightarrow \infty} g_n(\mathbf{r}_1, \dots, \mathbf{r}_n) = g_{n-1}(\mathbf{r}_1, \dots, \mathbf{r}_{n-1}), \tag{7}$$

$$i = 1, 2, \dots, n-1.$$

We shall assume (7) in later discussions.

It is convenient to define at this point the cluster functions f_n as follows:

$$g_1(\mathbf{r}_1) = f_1(\mathbf{r}_1) = 1, \tag{8}$$

$$g_2(\mathbf{r}_1, \mathbf{r}_2) = f_1(\mathbf{r}_1)f_2(\mathbf{r}_2) + f_2(\mathbf{r}_1, \mathbf{r}_2),$$

$$g_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = f_1(\mathbf{r}_1)f_1(\mathbf{r}_2)f_1(\mathbf{r}_3) + f_1(\mathbf{r}_1)f_2(\mathbf{r}_2, \mathbf{r}_3) + f_1(\mathbf{r}_2)f_2(\mathbf{r}_3, \mathbf{r}_1) + f_1(\mathbf{r}_3)f_2(\mathbf{r}_1, \mathbf{r}_2) + f_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3),$$

etc.

The structure of Eq. (8) is identical to that of the Ursell-Mayer expansion in classical statistical mechanics.¹⁰ We shall use the compact notation

$$\mathbf{g} = \alpha \mathbf{f} \quad \text{or} \quad \mathbf{f} = \alpha^{-1} \mathbf{g} \tag{8'}$$

to denote the structural relation (8) between any two sets of functions g_n and f_n .

The function f_n is symmetric in its n coordinates. The cluster condition (7) implies the following condition on f :

$$\lim_{r_{ij} \rightarrow \infty} f_n(r_1, \dots, r_n) = 0, \quad 1 \leq i < j \leq n. \tag{9}$$

Namely, f_n is significant only when the n particles are clustered together. Also it is easy to establish by induction that the sequential relation (6) implies the condition

$$\rho \int f_{n+1}(\mathbf{r}_1, \dots, \mathbf{r}_{n+1}) d\mathbf{r}_{n+1} = -nf_n(\mathbf{r}_1, \dots, \mathbf{r}_n). \tag{10}$$

We shall also need the Fourier transforms of the g and f functions:

$$G_n(\mathbf{k}_1, \dots, \mathbf{k}_n) = \rho^n \int g_n(\mathbf{r}_1, \dots, \mathbf{r}_n) \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \dots + \mathbf{k}_n \cdot \mathbf{r}_n)] d\mathbf{r}_1 \dots d\mathbf{r}_n, \tag{11}$$

$$F_n(\mathbf{k}_1, \dots, \mathbf{k}_n) = \rho^n \int f_n(\mathbf{r}_1, \dots, \mathbf{r}_n) \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \dots + \mathbf{k}_n \cdot \mathbf{r}_n)] d\mathbf{r}_1 \dots d\mathbf{r}_n.$$

With these definitions we now proceed to evaluate I_n . Substituting Eq. (2) into Eq. (3) and making use of the definition Eq. (11), one readily obtains the following:

$$I_1(\mathbf{k}_1) = G_1(\mathbf{k}_1),$$

$$I_2(\mathbf{k}_1, \mathbf{k}_2) = G_1(\mathbf{k}_1 + \mathbf{k}_2) + G_2(\mathbf{k}_1, \mathbf{k}_2),$$

$$I_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = G_1(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) + G_2(\mathbf{k}_1, \mathbf{k}_2 + \mathbf{k}_3) + G_2(\mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_1) + G_2(\mathbf{k}_3, \mathbf{k}_1 + \mathbf{k}_2) + G_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3), \tag{12}$$

etc.,

$$I_n(\mathbf{k}_1, \dots, \mathbf{k}_n) = \sum G_l \text{ (all distinct partitions of the } \mathbf{k}' \text{ s).}$$

A typical term of Eq. (12), e.g., $G_l(\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4 + \mathbf{k}_5, \dots)$, comes from the contribution in Eq. (3) when $\mathbf{r}_1 = \mathbf{r}_2, \mathbf{r}_3 = \mathbf{r}_4 = \mathbf{r}_5, \dots$, where l is the number of distinct \mathbf{r} 's. We shall use the compact notation

$$\mathbf{I} = \beta \mathbf{G} \quad \text{or} \quad \mathbf{G} = \beta^{-1} \mathbf{I} \tag{12'}$$

to denote the structural relation (12) between any two sets of functions I_n and G_n .

It is clear from the definitions (11), (8), and (8') that

$$\mathbf{G} = \alpha \mathbf{F}. \tag{13}$$

Hence, from (12'),

$$\mathbf{I} = \beta \alpha \mathbf{F}. \tag{14}$$

We now make use of the identity

$$\beta \alpha = \alpha \beta, \tag{15}$$

which can be proved by observing that every term in $\beta \alpha \mathbf{F}$ is in $\alpha \beta \mathbf{F}$ and vice versa. We then arrive at

$$\mathbf{I} = \alpha \mathbf{U}, \tag{16}$$

where

$$\mathbf{U} = \beta \mathbf{F}. \tag{17}$$

Equation (16) is our *main result*. Note that the derivation of Eq. (16) involves only the definitions of the g, f, G , and F functions and is therefore exact. The cluster condition of Eq. (7) has not been used in these discussions.

We now discuss properties of the U functions defined by (17) as implied by the sequential and the cluster properties (6) and (7). It is easy to see from Eqs. (10) and (11) that

$$F_{n+1}(\mathbf{k}_1, \dots, \mathbf{k}_n, 0) = -nF_n(\mathbf{k}_1, \dots, \mathbf{k}_n). \quad (18)$$

As a consequence of Eq. (18), one can establish the relation

$$U_n(\mathbf{k}_1, \dots, \mathbf{k}_n) = 0 \quad \text{if any } k_i = 0. \quad (19)$$

Equation (19) is, of course, a consequence of the sequential relation Eq. (6) and is therefore exact. For example, Eqs. (17) and (19) recover the identity

$$I_{n+1}(\mathbf{k}_1, \dots, \mathbf{k}_n, 0) = NI_n(\mathbf{k}_1, \dots, \mathbf{k}_n), \quad (20)$$

which is implied by the definition (3).

The cluster condition (9) has the important consequence that F_n defined by Eq. (11) is of the order of N . Furthermore, from the translational invariance of f_n we see that F_n vanishes unless $\mathbf{k}_1 + \dots + \mathbf{k}_n = 0$. Since each U function is a linear combination of single F functions, we conclude that

$$U_n(\mathbf{k}_1, \dots, \mathbf{k}_n) = \delta_{\mathbf{k}_1 + \dots + \mathbf{k}_n, 0} O(N). \quad (21)$$

In particular

$$U_1(\mathbf{k}) = \delta_{\mathbf{k}, 0} N. \quad (22)$$

It follows then that the leading contribution in I_n [Eq. (16)] comes from the terms containing the most number of nonvanishing momentum-conserving δ functions. That is, the leading contribution can be broken into product of lower I_n 's if there exist partial momentum conservations among the \mathbf{k} 's (the degenerate case). The degeneracy factor can be easily counted. For example,

$$\langle \Pi(\rho_{\mathbf{k}_1} \rho_{-\mathbf{k}_i})^{n_i} \rangle = \Pi_i n_i! [U_2(\mathbf{k}_i, -\mathbf{k}_i)]^{n_i} [1 + O(N^{-1})]. \quad (23)$$

This result was first derived by Jackson and Feenberg^{5,7} in an elaborate analysis using the generalized Kirkwood superposition approximation for g_n . Since only g_2 enters in the expression of U_2 , we see that, to the lead order in N , Eq. (23) is exact. Indeed, an alternate derivation¹¹ of Eq. (23) using the generating function technique does not involve the use of higher distribution functions. The exact result is generated by the superposition approximation because the latter satisfies the cluster condition (7). Another example of application of Eq. (16) is the evaluation of the following matrix element⁸ which enters in the theory of dispersion of phonons in liquid He⁴:

$$I_5(\mathbf{k}, 1, -\mathbf{k}-1, \mathbf{h}, -\mathbf{h}) = U_3(\mathbf{k}, 1, -\mathbf{k}-1)U_2(\mathbf{h}, -\mathbf{h}) \times [1 + O(N^{-1})], \quad kl | \mathbf{k} + 1 | \mathbf{h} \neq 0. \quad (24)$$

This integral was first evaluated by Lai, Sim, and Woo⁸ using convolution approximations to g_3, g_4 , and g_5 . It is now clear that only g_3 and g_2 enter on the right-hand side of Eq. (24) consistent to a recent remark by Feenberg.⁹ Finally we remark that if $\delta_{\mathbf{k}_1 + \dots + \mathbf{k}_n, 0}$ is the only nonvanishing momentum-conserving factor, then

$$I_n(\mathbf{k}_1, \dots, \mathbf{k}_n) = U_n(\mathbf{k}_1, \dots, \mathbf{k}_n). \quad (16')$$

III. EVALUATION OF U_n BY THE CONVOLUTION APPROXIMATION

In this section we evaluate the U functions defined by Eq. (17) using the convolution form $g_n^{(c)}$ for g_n . If we define

$$f^{(c)} = \alpha^{-1} \mathbf{g}^{(c)} \quad (25)$$

and let $F_n^{(c)}$ be the Fourier transform [Eq. (11)] of $f_n^{(c)}$, our goal is then to compute

$$U^{(c)} = \beta F^{(c)}. \quad (26)$$

First, we remark that since $g_n^{(c)}$ satisfies the sequential relation exactly, $U_n^{(c)}$ shall satisfy Eq. (19). In fact, our result, Eq. (34'), yields precisely

$$U_n^{(c)} \propto k_1 k_2 \dots k_n \text{ for small } k\text{'s and } n \geq 3. \quad (27)$$

In the ensuing discussions it is again convenient $U_n^{(c)}$ is quite accurate, at least in the small k regions. Any correction would be of higher than the n th power in k 's.

In the ensuing discussions it is again convenient to introduce a diagrammatic notation for algebraic expressions. Readers are referred to the basic conventions and definitions given in Sec. III of Ref. 4. The principal definitions and a few new additions¹² are now reviewed.

A graph is a collection of points with lines joining certain pairs of points. A *root* (or *root point*) is a point with a numeral label and is represented by an open circle. Unlabeled points are represented by solid, or black, circles. An *n-rooted* graph has precisely n root points, labeled from 1 to n . A *node* is a point having three or more incident lines. These lines *intersect* at the node point. A *terminal point* has only one line incident. The line incident to a terminal point will be called a *terminal line*. A *Cayley tree* is a connected graph containing no cycles, i.e., one cannot return to a point on a Cayley tree by following a sequence of lines.

To obtain the mathematical expression represented by a graph, one simply writes for each black point a factor $\rho \int d\mathbf{r}_k$, where k is taken to be the label of this black point, and for each line connecting two points labeled i and j writes a factor $f_2(|\mathbf{r}_i - \mathbf{r}_j|)$. Any isolated root point has a factor 1. With these conventions, the convolution form for g_n is⁴

$g_n^{(c)}(\mathbf{r}_1, \dots, \mathbf{r}_n)$ = the collection of all distinct n -rooted graphs consisting of *connected* and *disconnected* Cayley trees provided that each black point is a node. (28)

A moment's reflection using (25) and (28) now yields

$f_n^{(c)}(\mathbf{r}_1, \dots, \mathbf{r}_n)$ = the collection of all distinct *connected* n -rooted Cayley trees provided that each black point is a node. (29)

It is now possible to evaluate the Fourier transform $F_n^{(c)}$ of $f_n^{(c)}$. Since every term in $f_n^{(c)}$ is a Cayley tree, the result is quite simple and can be expressed in terms of the Fourier transform of $f_2 = g_2 - 1$,

$$u(k) = S(k) - 1 = \rho \int e^{ik \cdot r} [g_2(r) - 1] dr. \quad (30)$$

In fact, every term in $F_n^{(c)}(\mathbf{k}_1, \dots, \mathbf{k}_n)$ can also be conveniently represented by a graph related to the graph of $f_n^{(c)}$. The following further graph definitions will be useful.

A *normal* graph is one in which all roots are terminal points. Thus Fig. 1(b) is a normal graph while Fig. 1(a) is not. We speak of the following process which converts a graph into a normal one as the normalization of a graph. The normalization process is simply to remove the label of any nonterminal root point, thus leaving a black point, add a new root point with this label, and connect it to the black point by a *dotted* line. In this way the graph of Fig. 1(a) is normalized into that of Fig. 1(b). We see that a normalized graph will now have two kinds of lines, the solid and the dotted ones. The dotted lines are always terminal lines.

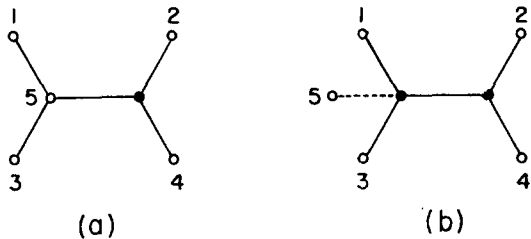


FIG. 1. Normalization of a graph [graph (a) is normalized into graph (b)].

Consider a given graph \mathcal{G} in $f_n^{(c)}$. We leave it for the readers to verify that the Fourier transform [Eq. (11)] of this graph can be obtained by the following rules:

1. Normalize \mathcal{G} if it contains nonterminal root points.
2. In the normalized graph label the terminal line (solid or dotted) connected to the i th root with momentum \mathbf{k}_i .
3. If all lines incident to a node are labeled except one, then label this remaining line with a momentum equal to the sum of all the previously labeled momenta surrounding this node.
4. Repeat 3 until all lines are labeled.

5. For each *solid* line labeled by \mathbf{k} write a factor $u(k)$. For each *dotted* line write a factor 1.
6. The Fourier transform of \mathcal{G} is the product of all factors in 5 and the factor $N\delta_{\mathbf{k}_1 + \dots + \mathbf{k}_n, 0}$.

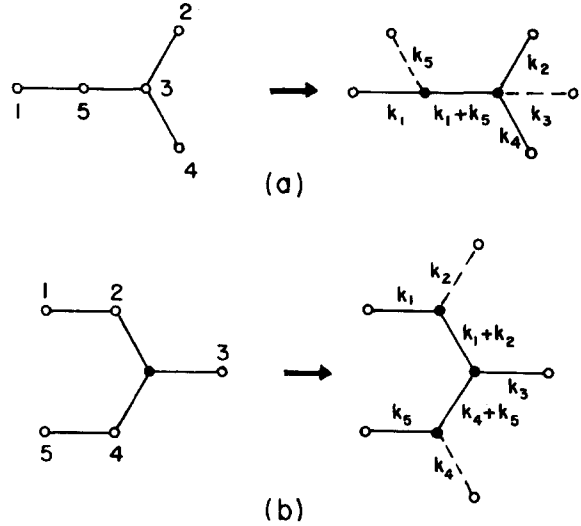


FIG. 2. Fourier transforms of two terms of $f_5^{(c)}$.

We remark that the momentum labelings are unique because the graphs are all Cayley trees and because the total momentum is conserved. Two examples are given in Fig. 2. The graphs on the left are two typical terms of $f_5^{(c)}$, while the graphs on the right are their Fourier transforms. Explicitly Fig. 2 says the following:

$$(a) \quad \rho^5 \int f_{15} f_{53} f_{23} f_{34} \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \dots + \mathbf{k}_5 \cdot \mathbf{r}_5)] \times d\mathbf{r}_1 \dots d\mathbf{r}_5 = Nu_1 u_{1+5} u_2 u_4 \delta_{1+2+3+4+5},$$

$$(b) \quad \rho^6 \int f_{12} f_{26} f_{36} f_{46} f_{45} \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \dots + \mathbf{k}_5 \cdot \mathbf{r}_5)] \times d\mathbf{r}_1 \dots d\mathbf{r}_6 = Nu_1 u_{1+2} u_3 u_{4+5} u_5 \delta_{1+2+3+4+5},$$

where we have adopted the shorthand notations

$$u_1 = u(\mathbf{k}_1), \quad u_{1+2} = u(|\mathbf{k}_1 + \mathbf{k}_2|) \quad (31)$$

$$\delta_{1+2} = \delta_{\mathbf{k}_1 + \mathbf{k}_2, 0}, \quad \text{etc.}$$

Thus we arrive at

$$F_n^{(c)}(\mathbf{k}_1, \dots, \mathbf{k}_n) = \text{the collection of all graphs of } f_n^{(c)} \text{ subject to the rules 1-6.} \quad (32)$$

$F_n^{(c)}$ for $n = 1, 2, 3, 4$ are given explicitly in Fig. 3, where only the topologically distinct graphs are shown and the momentum labels have been deleted.

It is seen from Fig. 3 that in the expression of $F_n^{(c)}$ there exist pairs of graphs which are identical except that in one graph a given terminal line is solid while in the other the same terminal line is dotted. We may then combine these two graphs into a single one so that this terminal line is doubled (solid and dotted lines). The weight of this

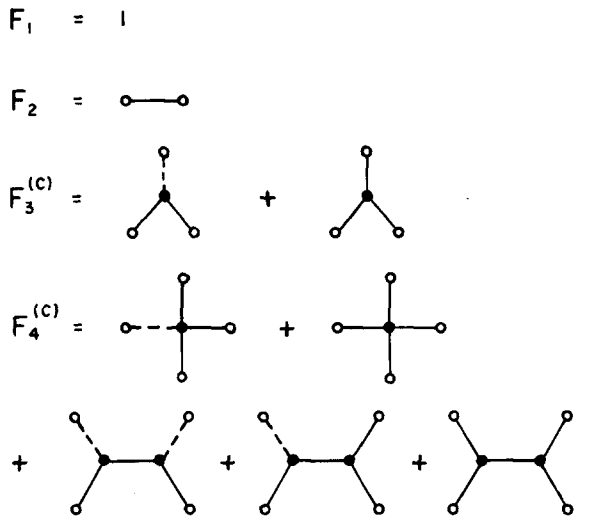


FIG. 3. Diagrammatic representations of $F_n^{(c)}$ for $n = 1, 2, 3, 4$.

double line is now $u(k) + 1 = S(k)$. However, we cannot do this simultaneously for two or more terminal lines intersecting at one node because according to our rules of normalization no graph has intersecting dotted lines. This problem is resolved when we substitute Eq. (32) into Eq. (26) to compute $U_n^{(c)}$. From the definition (12) or (12') we see that in some graphs of $U_n^{(c)}$ the terminal lines have momenta which are the sums of individual k_i 's. These graphs can be converted to have intersecting dotted lines and give rise to precisely those graphs we need. First a dotted terminal line having a momentum Σk_i can be split into several terminal lines, each having a label k_i . For a solid terminal line having a momentum Σk_i , one simply adds new terminal points and connects all these new points to the original terminal point by dotted lines. Three examples of such conversion for graphs $U_4^{(c)}$ are shown in Fig. 4. Consider

$$U_4^{(c)}(k_1, k_2, k_3, k_4) = \dots + F_2(k_1, k_2 + k_3 + k_4) + \dots + F_3^{(c)}(k_1, k_2, k_3 + k_4) + \dots$$

The graph of $F_2(k_1, k_2 + k_3 + k_4) = Nu_1 \delta_{1+2+3+4}$ is the one on the left in Fig. 4(a). By the above process this graph is converted to the one on the right in Fig. 4(a). The latter now has four root points with single momentum labels. Similarly, Fig. 4(b) denotes the same conversion for the term $Nu_2 u_{3+4} \delta_{1+2+3+4}$ in $F_3^{(c)}(k_1, k_2, k_3 + k_4)$, etc. Note that this process results in the same algebraic expression because of rule 3 above.

After converting all graphs of $U_n^{(c)}$ in Eq. (26) according to this rule, we see that

$$U_n^{(c)}(k_1, \dots, k_n) = \text{the collection of all distinct normal } n\text{-rooted Cayley trees provided that each black point is a node. The terminal lines can be either solid or dotted, each considered as distinct.} \quad (33)$$

Of course, rules 2-6 must be used in Eq. (33). The

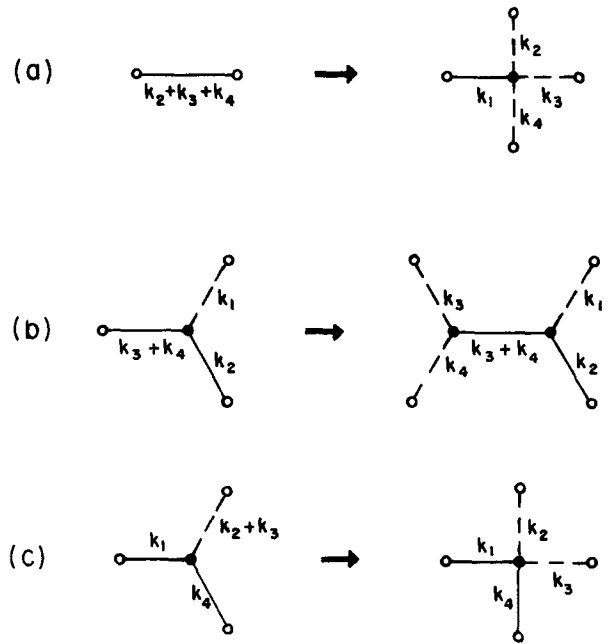


FIG. 4. Reduction of three graphs in $U_4^{(c)}$ to single momentum labels for the terminal lines

identity between Eqs. (33) and (26) can be established by observing that every graph in Eq. (26) is in Eq. (33) and vice versa.

It is now possible to combine the solid and dotted lines of all the terminal lines at the same time to form double lines. Thus we arrive at our final result:

$$U_n^{(c)}(k_1, \dots, k_n) = \text{the collection of all distinct normal } n\text{-rooted Cayley trees provided that each black point is a node. All terminal lines are double (solid and dotted) lines.} \quad (34)$$

Graphs for $U_n^{(c)}$ are shown in Fig. 5 for $n = 1, 2, 3, 4, 5$, where all momentum labels are deleted and

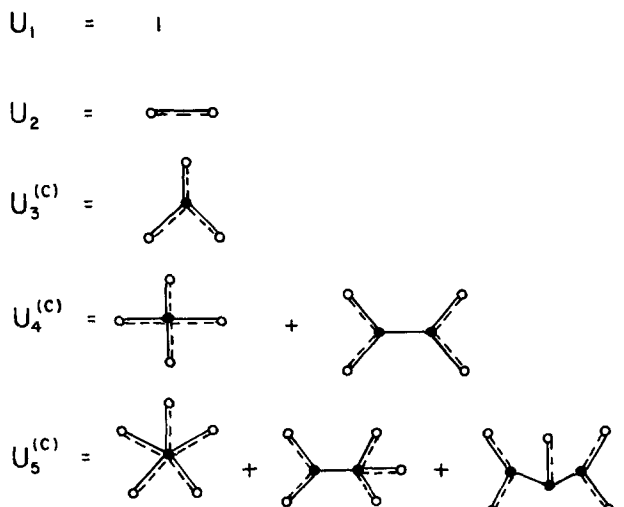


FIG. 5. Diagrammatic representations of $U_n^{(c)}$ for $n = 1, 2, 3, 4, 5$. The double lines have weights $S(k_i)$ while the single lines have weights $u(k)$ (see text).

only the topologically distinct graphs are shown. Again rules 2-6 must be used in Eq. (34) with the following addition to rule 5:

For each double terminal line with a label k write a factor $S(k)$.

Explicitly, Eq. (34) reads

$$U_2(\mathbf{k}_1, \mathbf{k}_2) = N\delta_{1+2}S_1,$$

$$U_n^{(c)}(\mathbf{k}_1, \dots, \mathbf{k}_n) = N\delta_{1+2+\dots+n}S_1 \dots S_n (1 + A_n), \quad n \geq 3 \quad (34')$$

with¹³

$$A_3 = 0,$$

$$A_4 = u_{1+2} + u_{1+3} + u_{1+4}, \quad (34'')$$

$$A_5 = \sum_{1 \leq i < j \leq 5} u_{i+j} + \sum_{1 \leq i < j < k \leq 5} u_{i+j+k}.$$

A_4 and A_5 can be read off from Fig. 5. In general, A_n is some linear combination of products of the u 's and can be represented by the diagrams in (34) with the terminal lines stripped. We note the factor $S_1 \dots S_n$ in $U_n^{(c)}$ for $n \geq 3$. Since in a liquid $S(k) \propto k$ for small k ,^{1,14} we arrive at Eq. (27), the result quoted earlier.

IV. ORTHONORMAL BASIS

One possible application of our result is the construction of orthonormal bases in the quantum theory of liquid He⁴. Jackson and Feenberg⁵ first considered this problem in the paired phonon space. We now briefly outline their result (with somewhat simplified analysis) and indicate the direction of possible extensions.

Consider the normalized $\pm \mathbf{k}$ phonon states

$$\psi_{l+s,l} = C_{l,s} \psi_0 \rho_k^{l+s} \rho_{-k}^l, \quad \text{for fixed integral } s, \quad (35)$$

where ψ_0 is the ground state wavefunction and the normalization constant $C_{l,s} = [NS(k)]^{-(l+2s)/2} \times$

$[(l+2s)!]^{-1/2}$ can be determined from Eq. (23).

We wish to construct the orthonormal set $|\hat{p}\rangle$ defined by the linear transformation

$$|\hat{p}\rangle = \sum_{l=0}^p a_{pl} \psi_{l+s,l}, \quad (36)$$

where for brevity the dependences of $|\hat{p}\rangle$ on s and a_{pl} have been deleted.

A convenient set of equations to work with is⁵

$$a_{pp} \langle \hat{p} | \psi_{h+s,h} \rangle = \delta_{hp}, \quad h \leq p. \quad (37)$$

Via Eq. (35) for $\psi_{h+s,h}$, Eq. (37) becomes

$$\sum_{l=0}^p a_{pp} a_{pl} \frac{(l+h+s)!}{[(2l+s)!(2h+s)!]^{1/2}} = \delta_{hp}, \quad h \leq p. \quad (38)$$

To solve Eq. (38), we define

$$a_{pp} a_{pl} = \frac{[(2l+s)!(2p+s)!]^{1/2}}{(l+s)!p!} \alpha_l \quad (39)$$

and multiply Eq. (38) by the factor $[(2h+s)!]^{1/2}/h!$. The result is the equation

$$\sum_{l=0}^p \binom{l+h+s}{h} \alpha_l = \delta_{hp}, \quad h \leq p. \quad (40)$$

Comparing Eq. (40) with the identity¹⁵

$$\sum_{l=0}^p (-1)^{l+p} \binom{p}{l} \binom{l+h+s}{h} = \delta_{ph}, \quad h \leq p, \quad (41)$$

we find

$$\alpha_l = (-1)^{l+p} \binom{p}{l}; \quad (42)$$

hence

$$a_{pl} = (-1)^{l+p} \left[\binom{p}{l} \binom{2l+s}{l} \binom{p+s}{l+s} \right]^{1/2}. \quad (43)$$

This completes the construction of the orthonormal set $|\hat{p}\rangle$ in the paired phonon space.

One direction of possible extensions is to construct an orthonormal basis using the n -phonon states

$$\psi_m^{(n)} = C_m \psi_0 (\rho_{\mathbf{k}_1} \dots \rho_{\mathbf{k}_n})^m, \quad m = 0, 1, 2, \dots, \quad (44)$$

where $\mathbf{k}_1 + \dots + \mathbf{k}_n = 0$. One can indeed carry out a similar analysis for finding the orthonormal basis

$$|\hat{p}\rangle = \sum_{l=0}^p a_{pl} \psi_l^{(n)}. \quad (45)$$

The resulting equation to solve turns out to be

$$\sum_{l=0}^p \binom{h+l}{h}^{n-1} \alpha_l = \delta_{hp}, \quad h \leq p, \quad (46)$$

where

$$\alpha_l = \left[\binom{2l}{l} \binom{2p}{p} \right]^{-(n-1)/2} a_{pp} a_{pl}.$$

Unfortunately, we have been unable to find the solution of this equation for $n \geq 3$. However, since our result shows that the two and higher phonon states are essentially independent in computing the matrix elements, it would be possible to include only a few $\psi_m^{(c)}$ for small values of m and n . This would then constitute an extension of the case $n = 3$ and $m = 0, 1$ considered by Davison and Feenberg.¹⁶

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$$(x - 1)^p x^{s+h} = \sum_{l=0}^p (-1)^{l+p} \binom{p}{l} x^{l+s+h}$$

 [see J. Riordan, *Combinatorial Identities* (Wiley, New York, 1968), p. 11]. We also remark that Eq. (41) is a generalization of one of the two binomial coefficient identities obtained by D. M. Rosenbaum, *J. Math. Phys.* **8**, 1973 (1967), and H. W. Gould, *J. Math. Phys.* **10**, 49 (1969). Their identity (B) corresponds to taking $h = p - 1$ in Eq. (41).
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Trapped Surfaces and the Development of Singularities*

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The study of singularities in general relativity was given a strong impetus by a topological approach due to Penrose and others, and powerful theorems concerning their existence have been developed. In particular a theorem by Penrose states that under certain conditions the existence of a trapped surface in a space-time guarantees that singularities will develop. Using the spin coefficient formalism we generalize from the Schwarzschild solution and prove the existence of a wide class of solutions possessing such trapped surfaces by displaying the solutions to terms linear in a certain null coordinate. Then, using an asymptotic procedure, the method is generalized to include a class of solutions possessing "asymptotically trapped surfaces."

1. INTRODUCTION

In 1965 Penrose presented a remarkable theorem on the existence space-time singularities which must follow from the existence of a trapped surface (a trapped surface being a compact spacelike 2-surface such that both sets of null rays orthogonal to the surface have negative divergence at every point of the surface).¹ From this theorem great interest in trapped surfaces has developed. The theorem requires the existence of a global Cauchy hypersurface (GCH). A GCH in a space-time M is a three-dimensional submanifold S in M such that any timelike curve in M without endpoint has one and only one point in common with S . The notion of a GCH is related to the Laplacian idea of determinism (that the entire future of the universe can be completely determined by knowing the positions and velocities of all particles in the universe at one time, i.e., on one three-dimensional spacelike submanifold) by the fact that the Laplacian idea of determinism requires the existence of a GCH. That is, if a GCH does not exist in M , then for any three-dimensional spacelike submanifold I that we choose as our "initial" hypersurface ("present" state of the universe) we will be able to find an event A to the future of I through which there pass nonspacelike, i.e., either timelike or null, curves which have

no event in common with I . In this situation we see that, loosely speaking, such nonspacelike curves can transmit information to A without that information having ever registered on I . Thus, in order to maintain the "classical" notion of determinism we must assume the existence of a GCH. The conclusions in Secs. 4 and 5 assume the existence of a GCH in the space-times discussed.

Previous to the Penrose theorem it was believed by many (for example, see Lifshitz and Khalatnikov²) that the necessary collapse to a singularity of spherically symmetric matter within the Schwarzschild radius was simply due to the high symmetry involved. The Penrose theorem, with its lack of symmetry assumptions, denies this simple explanation and, in the consideration of space-time singularities, shifts attention away from the symmetry properties of the situation, focusing instead on the existence of trapped surfaces for $r < 2M$. The Penrose theorem says that this, rather than the symmetry, is the crucial factor guaranteeing the eventual singularity at $r = 0$ for collapsing matter. The Schwarzschild solution presents us with a situation from which to generalize and thereby show the existence of a general class of solutions exhibiting such trapped surfaces and the attendant singularities.