

Multiple density correlation functions for inhomogeneous systems^{a)}

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In applying the method of correlated basis functions to inhomogeneous systems such as electrons in a solid, in systems bounded by surfaces, and in systems with impurities, matrix elements of multiple density fluctuation operators are needed. These are the multiple density correlation functions. We evaluate these functions in the convolution approximation and express them in usable forms.

I. INTRODUCTION

In variational calculations for interacting quantum liquids and solids, correlated wavefunctions have made some rather impressive contributions.^{1,2} While this is particularly true for calculations on homogeneous systems, recent progress in treating certain classes of surface problems³ encourages us to explore further the applicability of correlated wavefunctions to many inhomogeneous systems. Among those considered are surfaces of liquid ³He and nuclear matter, inhomogeneous electron liquids, impurities in solids, exciton droplets, and atomic systems.

By correlated wavefunctions, we mean wavefunctions which take into account the more important correlation effects. In particular, one could modify the Slater determinant, D , with a Jastrow factor,

$$\psi = D \prod_{i < j} f(\mathbf{r}_i, \mathbf{r}_j), \quad (1)$$

to account for pair correlations. If the pairwise interaction between the particles contains a strong repulsive core, $f(\mathbf{r}_i, \mathbf{r}_j)$ can be chosen to diminish rapidly with $r_{ij} \equiv |\mathbf{r}_i - \mathbf{r}_j|$. Thus the Jastrow factor $\prod_{i < j} f(\mathbf{r}_i, \mathbf{r}_j)$ serves to discourage overlap of the cores and makes the wavefunction much more realistic.

In the case of homogeneous systems, the elements of D are plane waves (with spin functions for fermions), and momentum is a good quantum number. The matrix elements connecting correlated wavefunctions involve simple Fourier transforms of $f(r_{ij})$ and Kronecker deltas. They are not easy to calculate, but are still manageable with the help of appropriate approximation schemes. For inhomogeneous systems, D represents antisymmetrized products of single particle wavefunctions. The matrix elements become more complicated. We intend to show in this paper that, at least in the convolution approximation, they can still be calculated and expressed in usable forms.

To be specific, we shall write down the relevant

equations for an inhomogeneous electron liquid and identify the required matrix elements.

In this model, we assume a static lattice structure for the ions, so that the ion variables reduce to constant lattice vectors \mathbf{R}_α , $\alpha = 1, 2, \dots, N$. There are N electrons moving in a volume Ω consistent with the lattice vectors \mathbf{R}_α . The electron coordinates are denoted by \mathbf{r}_i , $i = 1, 2, \dots, N$. The electron density is represented by a function $n(\mathbf{r})$, and the mean density is given by $\rho \equiv N/\Omega \equiv (1/\Omega) \int n(\mathbf{r}) d\mathbf{r}$. The Hamiltonian for the electron system is then given by

$$H = \sum_{i=1}^N h_i + \sum_{i < j}^N v(r_{ij}) - \frac{1}{2} N \rho v_0, \quad (2)$$

where

$$h_i = \frac{-\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}_i), \quad (3)$$

$$V(\mathbf{r}_i) = \sum_{\alpha=1}^N v(|\mathbf{r}_i - \mathbf{R}_\alpha|), \quad (4)$$

and

$$v(r) = e^2/r. \quad (5)$$

In Eq. (2) v_0 denotes the Fourier transform of the Coulomb potential in the long wavelength limit. Thus the last term in Eq. (2) takes out the electron self-energy.

Generalizing our earlier work⁴ on the homogeneous electron liquid, an appropriate variational wavefunction will still take the form (1), except that D now represents a determinant made up of Bloch function elements and spin functions. For simplicity, we make the approximation that $f(\mathbf{r}_i, \mathbf{r}_j)$ be central, and write

$$\psi = D \cdot \prod_{i < j}^N f(r_{ij}) \equiv D \cdot \left\{ \exp \sum_{i < j}^N \frac{1}{2} u(r_{ij}) \right\}, \quad (6)$$

$$= D \cdot \left[\exp \left(\frac{1}{4\Omega} \sum_{\mathbf{k}} u(k) (\rho_{\mathbf{k}} \rho_{-\mathbf{k}} - N) \right) \right], \quad (7)$$

where

$$\rho_{\mathbf{k}} = \sum_{i=1}^N \exp(ik \cdot \mathbf{r}_i), \quad (8)$$

and

$$u(k) = \int u(r) \exp(ik \cdot \mathbf{r}) d\mathbf{r}. \quad (9)$$

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With respect to such a correlated wavefunction we must now evaluate the energy expectation value,

$$\langle H \rangle = \sum_{i=1}^N \langle h_i \rangle + \sum_{\substack{i < j \\ i=1}} \langle v(r_{ij}) \rangle - \frac{1}{2} N \rho v_0, \quad (10)$$

where

$$\langle O \rangle = \frac{\sum_{\{o\}} \int \psi^* O \psi d\mathbf{r}_1 \cdots d\mathbf{r}_N}{\sum_{\{o\}} \int \psi^* \psi d\mathbf{r}_1 \cdots d\mathbf{r}_N} \quad (11)$$

for any operator O . After several steps of integration by parts and algebraic manipulation, we find

$$\langle H \rangle = \sum_{i=1}^N \epsilon_i - \frac{\hbar^2}{8m\Omega^2} \sum_{\mathbf{k}, 1} u(k) u(l) \mathbf{k} \cdot \mathbf{l} \langle \rho_{\mathbf{k}} \rho_{\mathbf{l}} \rho_{-\mathbf{k}-\mathbf{l}} \rangle + \frac{1}{2\Omega} \sum_{\mathbf{k} \neq 0} v_{\mathbf{k}} (\langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle - N), \quad (12)$$

where $v_{\mathbf{k}} = 4\pi e^2/k^2$ and ϵ_i denotes the single particle energy given by

$$h\varphi_i(\mathbf{r}) = \epsilon_i \varphi_i(\mathbf{r}). \quad (13)$$

Clearly, we need the matrix elements

$$I_2(\mathbf{k}_1, \mathbf{k}_2) \equiv \langle \rho_{\mathbf{k}_1} \rho_{\mathbf{k}_2} \rangle, \quad (14)$$

and

$$I_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \equiv \langle \rho_{\mathbf{k}_1} \rho_{\mathbf{k}_2} \rho_{\mathbf{k}_3} \rangle, \quad (15)$$

for use in the energy formulas.

These matrix elements are many-body integrals. From classical statistical mechanics one learns how they might be evaluated with cluster expansion procedures or stochastic methods. Yet, to our taste, integral equation techniques appear more efficient and reliable. By generalizing the formalism developed in Ref. 4, we define

$$I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu) \equiv \langle \rho_{\mathbf{k}_1} \rho_{\mathbf{k}_2} \dots \rho_{\mathbf{k}_n} \rangle_{\mu}, \quad (16)$$

where the expectation value is now taken with respect to the wavefunction

$$\psi_{\mu} = D \cdot \left\{ \exp \sum_{i < j}^N \frac{\mu}{2} u(r_{ij}) \right\}. \quad (17)$$

Differentiating Eq. (16) with respect to μ , we find the recurrence relation

$$\begin{aligned} \frac{d}{d\mu} I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu) &= \frac{1}{2\Omega} \sum_{\mathbf{k}} u(k) [I_{n+2}(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n, \mathbf{k}, -\mathbf{k} | \mu) \\ &\quad - I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu) I_2(\mathbf{k}, -\mathbf{k} | \mu)], \end{aligned} \quad (18)$$

thus a hierarchy of differential equations. By truncating the hierarchy with a reasonable closure approximation, one can in principle solve the equations and obtain all $I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu)$, and in particular all

$$I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n) \equiv I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu = 1). \quad (19)$$

In the lowest orders, Eq. (18) yields

$$\begin{aligned} \frac{d}{d\mu} I_1(\mathbf{k}_1 | \mu) &= \frac{1}{2\Omega} \sum_{\mathbf{k}} u(k) [I_3(\mathbf{k}_1, \mathbf{k}, -\mathbf{k} | \mu) \\ &\quad - I_1(\mathbf{k}_1 | \mu) I_2(\mathbf{k}, -\mathbf{k} | \mu)] \\ \frac{d}{d\mu} I_2(\mathbf{k}_1, \mathbf{k}_2 | \mu) &= \frac{1}{2\Omega} \sum_{\mathbf{k}} u(k) [I_4(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}, -\mathbf{k} | \mu) \end{aligned}$$

$$- I_2(\mathbf{k}_1, \mathbf{k}_2 | \mu) I_2(\mathbf{k}, -\mathbf{k} | \mu)]. \quad (20)$$

If I_3 and I_4 are expressed in terms of I_1 and I_2 , then Eq. (20) is a set of two coupled differential equations and can be solved for $I_1(\mathbf{k} | \mu)$ and $I_2(\mathbf{k}_1, \mathbf{k}_2 | \mu)$.

In this paper, we derive general formulas for the matrix elements $I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu)$ which, in the convolution approximation are given in terms of I_1 and I_2 . Specific expressions for I_2, I_3 , and I_4 are given. Except where noted, the model in mind will be the inhomogeneous electron liquid as defined in this section. Detailed application and results will be presented elsewhere.

II. MATHEMATICAL FORMULATION

Consider an N -particle system which possesses a nonuniform density distribution. The inhomogeneity may be the consequence of an external periodic potential such as in the case of electron liquids in solids. It may also be caused by the existence of a surface, or the presence of local impurities. We shall first formulate our analysis generally without specifying the type of inhomogeneity to encompass all these possibilities. The result will then be specialized to the case of a periodic inhomogeneity.

As mentioned in the Introduction, we wish to evaluate the multiple density correlation function

$$I_n(\mathbf{k}_1, \dots, \mathbf{k}_n | \mu) = \langle \rho_{\mathbf{k}_1} \dots \rho_{\mathbf{k}_n} \rangle_{\mu}, \quad (21)$$

where $\langle \rangle_{\mu}$ denotes the quantum mechanical expectation value defined in Eq. (11) by the wavefunction $\psi_{\mu}(\mathbf{r}_1, \dots, \mathbf{r}_N)$ of the N -particle system. For convenience, we shall omit the subscript μ as well as all references to spins in the following.

The formal evaluation of I_n follows closely that for a homogeneous system.⁵ First, we define the n -particle distribution function

$$\begin{aligned} p_n(\mathbf{r}_1, \dots, \mathbf{r}_n) &= \frac{N!}{(N-n)!} \int |\psi|^2 d\mathbf{r}_{n+1} \dots d\mathbf{r}_N / \int |\psi|^2 d\mathbf{r}_1 \dots d\mathbf{r}_N, \end{aligned} \quad (22)$$

which, by definition, is symmetric in its n coordinates. For a homogeneous system the one-particle distribution function $p_1(\mathbf{r})$ is a constant equal to the mean particle density $\rho = N/\Omega$. For an inhomogeneous system $p_1(\mathbf{r})$ will be dependent on spatial coordinates. Next we define the cluster functions f_2, f_3, \dots , as follows:

$$\begin{aligned} p_2(\mathbf{r}_1, \mathbf{r}_2) &= p_1(\mathbf{r}_1) p_1(\mathbf{r}_2) [1 + f_2(\mathbf{r}_1, \mathbf{r}_2)], \\ p_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) &= p_1(\mathbf{r}_1) p_1(\mathbf{r}_2) p_1(\mathbf{r}_3) [1 + f_2(\mathbf{r}_1, \mathbf{r}_2) + f_2(\mathbf{r}_2, \mathbf{r}_3) \\ &\quad + f_2(\mathbf{r}_3, \mathbf{r}_1) + f_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)], \end{aligned} \quad (23)$$

etc.

Further, define the Fourier transforms:

$$\pi(\mathbf{k}) = \int p_1(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}) d\mathbf{r}, \quad (24)$$

$$p_1(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{k}} \pi(\mathbf{k}) \exp(-i\mathbf{k} \cdot \mathbf{r}), \quad (25)$$

$$F_n(\mathbf{k}_1, \dots, \mathbf{k}_n)$$

$$= \int p_1(\mathbf{r}_1) \dots p_1(\mathbf{r}_n) f_n(\mathbf{r}_1, \dots, \mathbf{r}_n) \times \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \dots + \mathbf{k}_n \cdot \mathbf{r}_n)] d\mathbf{r}_1 \dots d\mathbf{r}_n, \quad n \geq 2. \quad (26)$$

It is then a direct consequence of these definitions that the expectation value (21) can be written as⁵

$$I_1(\mathbf{k}) = \pi(\mathbf{k}),$$

$$I_2(\mathbf{k}_1, \mathbf{k}_2) = \pi(\mathbf{k}_1)\pi(\mathbf{k}_2) + U_2(\mathbf{k}_1, \mathbf{k}_2), \quad (27)$$

$$I_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = \pi(\mathbf{k}_1)\pi(\mathbf{k}_2)\pi(\mathbf{k}_3) + \pi(\mathbf{k}_1)U_2(\mathbf{k}_2, \mathbf{k}_3) + \pi(\mathbf{k}_2)U_2(\mathbf{k}_3, \mathbf{k}_1) + \pi(\mathbf{k}_3)U_2(\mathbf{k}_1, \mathbf{k}_2) + U_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3),$$

etc.,

where

$$U_2(\mathbf{k}_1, \mathbf{k}_2) = \pi(\mathbf{k}_1 + \mathbf{k}_2) + F_2(\mathbf{k}_1, \mathbf{k}_2),$$

$$U_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = \pi(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) + F_2(\mathbf{k}_1, \mathbf{k}_2 + \mathbf{k}_3) + F_2(\mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_1) + F_2(\mathbf{k}_3, \mathbf{k}_1 + \mathbf{k}_2) + F_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3), \quad (28)$$

etc.

This completes the formal evaluation of I_n . While Eqs. (27) and (28) are exact, the usefulness of this formulation rests in the fact that $U_n(\mathbf{k}_1, \dots, \mathbf{k}_n)$ assumes a simple form when the convolution approximation is used for p_n . This will then make the evaluation of I_n practical for reasonably large values of n . The rest of this paper will be devoted to evaluating U_n . However, there also exist some general properties of the F and U functions which are exact. We now describe these properties.

An immediate consequence of the definition (22) of p_n is the sequential relation⁵

$$\int p_1(\mathbf{r}) d\mathbf{r} = N, \quad (29)$$

$$\int p_{n+1}(\mathbf{r}_1, \dots, \mathbf{r}_{n+1}) d\mathbf{r}_{n+1} = (N-n)p_n(\mathbf{r}_1, \dots, \mathbf{r}_n), \quad n \geq 1. \quad (30)$$

Equations (29) and (30) imply, in turn, the following conditions on f_n :

$$\int p_1(\mathbf{r}_2) f_2(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_2 = -1, \quad (31)$$

$$\int p_1(\mathbf{r}_{n+1}) f_{n+1}(\mathbf{r}_1, \dots, \mathbf{r}_{n+1}) d\mathbf{r}_{n+1} = -n f_n(\mathbf{r}_1, \dots, \mathbf{r}_n), \quad n \geq 2. \quad (32)$$

Note that Eq. (31), which reflects the normalization of f_2 , is a rather stringent condition. It will play an essential role in later discussions.

In terms of the F functions, conditions (31) and (32) lead to

$$F_2(\mathbf{k}_1, 0) = -\pi(\mathbf{k}_1), \quad (33)$$

$$F_{n+1}(\mathbf{k}_1, \dots, \mathbf{k}_n, 0) = -n F_n(\mathbf{k}_1, \dots, \mathbf{k}_n). \quad (34)$$

It then follows from Eq. (28) that

$$U_n(\mathbf{k}_1, \dots, \mathbf{k}_n) = 0 \text{ for any } k_i = 0, \quad n \geq 2. \quad (35)$$

Equation (35) is an exact result, and is a direct consequence of the sequential relation. Assuming reasonable behavior for U_n , we then expect U_n to go to zero smoothly for small k_i . In fact, we shall explicitly see that under the convolution approximation of p_n which preserves the sequential relation, U_n vanishes linearly in k_i . However, it must be pointed out that it is not generally true that U_n is continuous at $k_i = 0$ such as in

the case of a short-range Jastrow function with $D = 1$. For such systems U_n will not vanish in the $k_i \rightarrow 0$ limit.

Another consequence of the definitions is that the function U_n is of the order of N .⁵ This is so because the moving of one particle to infinity reduces the n -particle distribution function to $(n-1)$ -particle distribution function. As a consequence, we expect

$$\lim_{r_i \rightarrow \infty} f_n(\mathbf{r}_1, \dots, \mathbf{r}_n) = 0, \quad 1 \leq i < j \leq n. \quad (36)$$

The assertion then follows from Eqs. (28) and (26). Similarly we expect $\pi(\mathbf{k})$ to be of the order of N if it does not vanish.

It proves convenient to introduce the Fourier transforms

$$\theta(\mathbf{K}_1, \mathbf{K}_2) = \frac{1}{\Omega^2} \int f_2(\mathbf{r}_1, \mathbf{r}_2) \exp[-i(\mathbf{K}_1 \cdot \mathbf{r}_1 + \mathbf{K}_2 \cdot \mathbf{r}_2)] d\mathbf{r}_1 d\mathbf{r}_2,$$

or

$$f_2(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\mathbf{K}_1, \mathbf{K}_2} \theta(\mathbf{K}_1, \mathbf{K}_2) \exp[i(\mathbf{K}_1 \cdot \mathbf{r}_1 + \mathbf{K}_2 \cdot \mathbf{r}_2)]. \quad (37)$$

It is easily verified that the normalization condition (31) of f_2 can be written as

$$\sum_{\mathbf{K}_2} \pi(\mathbf{K}_2) \theta(\mathbf{K}_1, \mathbf{K}_2) = -\delta_{\mathbf{K}_1}(\mathbf{K}_1, 0), \quad (38)$$

where $\delta_{\mathbf{K}_1}$ is the Kronecker delta function. The following identities implied by Eq. (38) will be used in later discussions:

$$\pi(\mathbf{k}) = \sum_{\mathbf{K}_1, \mathbf{K}_2} \pi(\mathbf{K}_1) \pi(\mathbf{k} + \mathbf{K}_2) [-\theta(\mathbf{K}_1 - \mathbf{k}, \mathbf{K}_2 + \mathbf{k})], \quad (39)$$

$$\pi(\mathbf{k}_1 + \mathbf{k}_2) = \sum_{\mathbf{K}_1, \mathbf{K}_2} \pi(\mathbf{k}_1 + \mathbf{K}_1) \pi(\mathbf{k}_2 + \mathbf{K}_2) [-\theta(\mathbf{K}_1 - \mathbf{k}_2, \mathbf{K}_2 + \mathbf{k}_2)]. \quad (40)$$

Despite its apparent asymmetric appearance, Eq. (40) is actually symmetric in \mathbf{k}_1 and \mathbf{k}_2 .

III. CONVOLUTION APPROXIMATION

In the development of the theory of liquid ⁴He, Jackson and Feenberg⁶ proposed a convolution approximation for the three-particle distribution function, p_3 , which satisfies the sequential relation exactly. The convolution form has since been extended to p_n for general n ,⁷ and used in the evaluation of I_n for a homogeneous system.⁵ To evaluate I_n for inhomogeneous systems, we shall therefore first need a generalization of the convolution approximation.

It is straightforward to generalize the convolution form for p_3 . Using Eq. (31), one easily verifies that the expression

$$p_3^{(c)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = p_1(\mathbf{r}_1) p_1(\mathbf{r}_2) p_1(\mathbf{r}_3) [1 + f_{12} + f_{23} + f_{31} + f_{12} f_{23} + f_{23} f_{31} + f_{31} f_{12} + \int p_1(\mathbf{r}_4) f_{14} f_{24} f_{34} d\mathbf{r}_4] \quad (41)$$

satisfies the sequential relation Eq. (30) for $n = 2$.

Here, we have adopted the shorthand notation

$$f_{ij} = f_2(\mathbf{r}_i, \mathbf{r}_j).$$

Since Eq. (41) reduces to the convolution form for p_3

$$p_3^{(c)} = 1 + \begin{array}{c} 1 \\ \circ \\ | \\ \circ \\ 2 \end{array} + \begin{array}{c} 2 \\ \circ \\ | \\ \circ \\ 3 \end{array} + \begin{array}{c} 3 \\ \circ \\ | \\ \circ \\ 1 \end{array} + f_3^{(c)}$$

$$f_3^{(c)} = \begin{array}{c} 2 \\ \circ \\ / \quad \backslash \\ \circ \quad \circ \\ 1 \quad 3 \end{array} + \begin{array}{c} 3 \\ \circ \\ / \quad \backslash \\ \circ \quad \circ \\ 2 \quad 1 \end{array} + \begin{array}{c} 1 \\ \circ \\ / \quad \backslash \\ \circ \quad \circ \\ 3 \quad 2 \end{array} + \begin{array}{c} 1 \\ \circ \\ | \\ \bullet \\ | \\ \circ \\ 2 \end{array}$$

FIG. 1. Graphical representation of $p_3^{(c)}$.

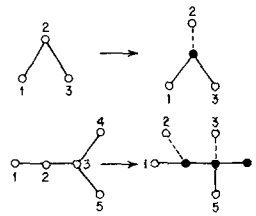


FIG. 3. Examples of graph normalization.

of Refs. 6 and 7 upon taking $p_1(\mathbf{r}) = \rho$, it is a natural generalization of the convolution approximation.

To further generalize Eq. (41) to $p_n^{(c)}$ for $n > 3$, it is convenient, as in Ref. 7, to use graphical terms for algebraic expressions.

We refer to Ref. 7 for definitions of terms in linear graph theory. It is seen that Eq. (41) can be represented by precisely the same graphs as in Ref. 7, which we reproduce in Fig. 1. However, the following rules will now be used to convert graphs into algebraic expressions:

- (i) The line joining two root points labeled i and j carries a weight f_{ij} .
- (ii) The root point labeled i carries a weight $p_1(\mathbf{r}_i)$.
- (iii) Each black point carries a dummy label k and a weight

$$\int p_1(\mathbf{r}_k) d\mathbf{r}_k.$$

- (iv) The algebraic expression represented by a graph is the product of the weights in (i)–(iii).

With the diagram rules (i)–(iv), it is not difficult to see that the analysis of Ref. 7 can be carried through without change. The key step is, of course, the utilization of the normalization condition (31). The consideration eventually leads to the same expression of $p_n^{(c)}$ as in Ref. 7.

For our purpose, it suffices to give only the expression for f_n . One finds as in Ref. 7

$$[\prod_i p_i(\mathbf{r}_i)] f_n^{(c)}(\mathbf{r}_1, \dots, \mathbf{r}_n) \quad (42)$$

= the collection of all distinct, connected, n -rooted Cayley trees, provided that all black points are nodes.

As an example, $f_3^{(c)}$ is shown in Fig. 1.

We now substitute Eq. (42) into Eq. (26) to evaluate $F_n^{(c)}$, the convolution form for F_n . The result is most conveniently expressed in terms of the Fourier transformed functions $\pi(\mathbf{k})$ and $\theta(\mathbf{K}_1, \mathbf{K}_2)$. The substitution leads to

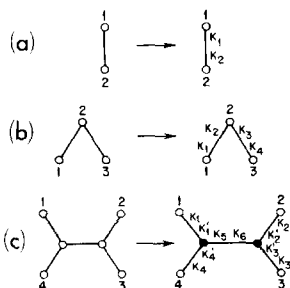


FIG. 2. Graphical representations of expressions (45)–(47).

$$F_n^{(c)}(\mathbf{k}_1, \dots, \mathbf{k}_n) = \text{the same graphs as in Eq. (42),} \quad (43)$$

provided that the following graph rules are used:

- (a) Cut each line into two halves at the midpoint and label the two halves with momenta \mathbf{K}_α and \mathbf{K}_β respectively.

- (b) The line labeled \mathbf{K}_α and \mathbf{K}_β carries a weight

$$\sum_{\mathbf{K}_\alpha, \mathbf{K}_\beta} \theta(\mathbf{K}_\alpha, \mathbf{K}_\beta). \quad (44)$$

- (c) The root point labeled i carries a weight $\pi(\mathbf{k}_i + \sum \mathbf{K}_\alpha)$, where $\sum \mathbf{K}_\alpha$ is the sum of the momenta of the half-lines incident at the root point.

- (d) Each black point carries a weight $\pi(\sum \mathbf{K}_\alpha)$, where $\sum \mathbf{K}_\alpha$ has the same meaning as in (c).

- (e) The algebraic expression of a graph in Eq. (43) is the product of all the weights in (b)–(d).

Note that we have numbered the momentum-space graph rules by Roman letters to distinguish them from the rules in the \mathbf{r} -space. Some typical terms in Eq. (43) are shown in Fig. 2 with the algebraic expressions given as follows:

$$\begin{aligned} \text{(a)} \quad & F_2(\mathbf{k}_1, \mathbf{k}_2) \\ &= \int p_1(\mathbf{r}_1) p_1(\mathbf{r}_2) f_2(\mathbf{r}_1, \mathbf{r}_2) \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \mathbf{k}_2 \cdot \mathbf{r}_2)] d\mathbf{r}_1 d\mathbf{r}_2 \\ &= \sum_{\mathbf{K}_1, \mathbf{K}_2} \pi(\mathbf{k}_1 + \mathbf{K}_1) \pi(\mathbf{k}_2 + \mathbf{K}_2) \theta(\mathbf{K}_1, \mathbf{K}_2), \end{aligned} \quad (45)$$

$$\begin{aligned} \text{(b)} \quad & \int p_1(\mathbf{r}_1) p_1(\mathbf{r}_2) p_1(\mathbf{r}_3) f_{12} f_{23} \\ & \times \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \mathbf{k}_2 \cdot \mathbf{r}_2 + \mathbf{k}_3 \cdot \mathbf{r}_3)] d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \\ &= \sum_{\mathbf{K}_1, \dots, \mathbf{K}_4} \pi(\mathbf{k}_1 + \mathbf{K}_1) \pi(\mathbf{k}_2 + \mathbf{K}_2 + \mathbf{K}_3) \pi(\mathbf{k}_3 + \mathbf{K}_4) \\ & \times \theta(\mathbf{K}_1, \mathbf{K}_2) \theta(\mathbf{K}_3, \mathbf{K}_4), \end{aligned} \quad (46)$$

$$\begin{aligned} \text{(c)} \quad & \int p_1(\mathbf{r}_1) \dots p_6(\mathbf{r}_6) f_{15} f_{45} f_{26} f_{36} f_{56} \\ & \times \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \dots + \mathbf{k}_6 \cdot \mathbf{r}_6)] d\mathbf{r}_1 \dots d\mathbf{r}_6 \\ &= \sum_{\mathbf{K}_i} \sum_{\mathbf{K}'_i} [\prod_{i=1}^4 \pi(\mathbf{k}_i + \mathbf{K}_i) \theta(\mathbf{K}_i, \mathbf{K}'_i)] \theta(\mathbf{K}_5, \mathbf{K}_6) \\ & \times \pi(\mathbf{K}'_1 + \mathbf{K}'_4 + \mathbf{K}_5) \pi(\mathbf{K}'_2 + \mathbf{K}'_3 + \mathbf{K}_6). \end{aligned} \quad (47)$$

We are now in a position to evaluate $U_n^{(c)}$ by combining Eqs. (43) and (28). To this end it is convenient to introduce the normal graphs as in Ref. 5. Whenever a rooted point, labeled i , say, occurs as an interior point, the graph is "normalized" by converting the root point into a black point, adding a new root point with the same label i , and connecting the new root point to

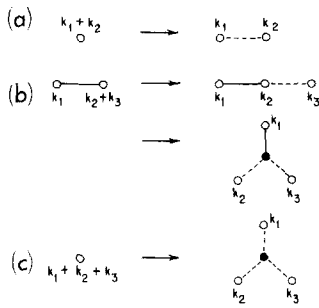


FIG. 4. Examples of graph normalization where the momentum label is the sum of individual momenta.

the black point by a broken line. Some examples of this normalization procedure are shown in Fig. 3. Although a new (broken) line and a new point are added to the graph, the graph weight can be made unchanged if we use identity (39), and associate with a broken line the weight

$$-\sum_{\mathbf{K}_1, \mathbf{K}_2} \theta(\mathbf{K}_1 - \mathbf{k}_i, \mathbf{K}_2 + \mathbf{k}_i). \quad (48)$$

Here the diagram rules (a)–(e) are followed except that the weight (48) is used in place of (44) for broken lines. In (48), \mathbf{K}_2 is the momentum label of the half-dashed line incident to the new root point.

The above normalization procedure can be applied in succession to graphs whose labels are sums of individual momenta. Some examples are shown in Fig. 4. Here, Fig. 4(a) is precisely the graphical representation of identity (40); Fig. 4(c) reads

$$\begin{aligned} &\pi(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) \\ &= \sum_{\mathbf{K}_i, \mathbf{K}'_i} \left\{ \prod_{i=1}^3 \pi(\mathbf{k}_i + \mathbf{K}_i) [-\theta(\mathbf{K}'_i - \mathbf{k}_i, \mathbf{K}_i + \mathbf{k}_i)] \right\} \\ &\quad \times \pi(\mathbf{K}'_1 + \mathbf{K}'_2 + \mathbf{K}'_3). \end{aligned} \quad (49)$$

An expression for Fig. 4(b) can be similarly obtained from the graph using the rules (a)–(e).

After all graphs in Eq. (43) are normalized, we arrive at

$$\begin{aligned} &U_n^{(c)}(\mathbf{k}_1, \dots, \mathbf{k}_n) \\ &= \text{the collection of all distinct normal } n\text{-rooted} \\ &\text{Cayley trees whose black points are nodes. The terminal} \\ &\text{lines are either solid or broken.} \end{aligned} \quad (50)$$

(Terminal lines are the lines incident to the root points which are now on the surface of the Cayley tree.) Now, each terminal line is either solid or broken, irrespective of the condition on other lines; we may therefore combine the solid and broken lines to form a double terminal line and obtain

$$\begin{aligned} &U_n^{(c)}(\mathbf{k}_1, \dots, \mathbf{k}_n) \\ &= \text{the collection of all distinct normal } n\text{-rooted} \\ &\text{Cayley trees whose black points are nodes and whose} \\ &\text{terminal lines are double lines.} \end{aligned} \quad (51)$$

The double (terminal) line now carries a weight which is given by combining Eq. (44) and (48),

$$\sum_{\mathbf{K}_1, \mathbf{K}_2} [\theta(\mathbf{K}_1, \mathbf{K}_2) - \theta(\mathbf{K}_1 - \mathbf{k}_i, \mathbf{K}_2 + \mathbf{k}_i)]. \quad (52)$$

Here, as in Eq. (48), \mathbf{K}_2 is the momentum of the half-double line incident to the root point labeled i .

Equation (51) is identical to the result of Ref. 5,

except that the graph rules are now (a)–(e) with Eq. (52) in place of Eq. (44) for terminal lines. Graphs for $U_n^{(c)}$ have been given in Fig. 5 of Ref. 5 for $n \leq 5$. We give here only the explicit expression for $n = 2, 3, 4$:

$$\begin{aligned} U_2(k_1, k_2) &= \sum_{\mathbf{K}_1, \mathbf{K}_2} \pi(\mathbf{K}_1 + \mathbf{k}_1) \pi(\mathbf{K}_2 + \mathbf{k}_2) \\ &\quad \times [\theta(\mathbf{K}_1, \mathbf{K}_2) - \theta(\mathbf{K}_1 - \mathbf{k}_2; \mathbf{K}_2 + \mathbf{k}_2)], \end{aligned} \quad (53)$$

$$\begin{aligned} U_3^{(c)}(k_1, k_2, k_3) &= \sum_{\mathbf{K}_i, \mathbf{K}'_i} \pi(\mathbf{K}'_1 + \mathbf{K}'_2 + \mathbf{K}'_3) \prod_{i=1}^3 \{ \pi(\mathbf{K}_i + \mathbf{k}_i) \\ &\quad \times [\theta(\mathbf{K}'_i, \mathbf{K}_i) - \theta(\mathbf{K}'_i - \mathbf{k}_i, \mathbf{K}_i + \mathbf{k}_i)] \}, \end{aligned} \quad (54)$$

$$\begin{aligned} &U_4^{(c)}(k_1, k_2, k_3, k_4) \\ &= \sum_{\mathbf{K}_i, \mathbf{K}'_i} \prod_{i=1}^4 \{ \pi(\mathbf{K}_i + \mathbf{k}_i) [\theta(\mathbf{K}'_i, \mathbf{K}_i) \\ &\quad - \theta(\mathbf{K}'_i - \mathbf{k}_i, \mathbf{K}_i + \mathbf{k}_i)] \} [\pi(\mathbf{K}'_1 + \mathbf{K}'_2 + \mathbf{K}'_3 + \mathbf{K}'_4) \\ &\quad + \pi(\mathbf{K}'_1 + \mathbf{K}'_2 + \mathbf{K}_5) \pi(\mathbf{K}'_3 + \mathbf{K}'_4 + \mathbf{K}_6) \theta(\mathbf{K}_5, \mathbf{K}_6)]. \end{aligned} \quad (55)$$

Note that Eq. (52) implies $U_n^{(c)} \sim k_i$ for any $k_i \sim 0$ if the function θ has a Taylor's expansion. This is the result alluded to earlier in the text.

IV. APPLICATIONS

The expression (51) for U_n has been derived using the convolution approximation; otherwise it is an exact result. In applications further simplification usually arises either due to some special properties of the physical system or additional approximations introduced for convenience. To make our formulation useful we now describe some of these simplifications.

Consider first the case of a homogeneous system. For an isotropic and homogeneous many-particle system we expect $\rho_1(\mathbf{r}) = \rho$ and the two-particle distribution function $\rho_2(\mathbf{r}_1, \mathbf{r}_2)$ to depend only on the distance between the two particles, or

$$f_2(\mathbf{r}_1, \mathbf{r}_2) = h(r_{12}). \quad (56)$$

Thus from Eq. (37) we find

$$\theta(\mathbf{K}_1, \mathbf{K}_2) = N^{-1} u(K_1) \delta_{\mathbf{K}_r}(\mathbf{K}_1 + \mathbf{K}_2, 0), \quad (57)$$

where

$$u(k) = \rho \int \exp(i\mathbf{k} \cdot \mathbf{r}) h(r) d\mathbf{r}. \quad (58)$$

The normalization condition now reads

$$u(0) = -1. \quad (59)$$

Also from Eq. (25),

$$\pi(\mathbf{k}) = N \delta_{\mathbf{K}_r}(\mathbf{k}, 0). \quad (60)$$

Substituting these results into Eq. (51), we see that the graph rules (a)–(e) may be greatly simplified. In particular, each line now carries a single momentum label and a weight $u(\mathbf{K})$ for internal lines and weight $u(k_i) - u(0)$ for terminal lines. The root and black points carry no weight except that momentum is conserved at black points. This is the result of Ref. 7.

In the application to inhomogeneous systems it may be necessary for reasons of practicality to assume approximation (56), even though the one-particle distribution function should still be dependent on spatial

coordinates. Again, this leads to a single momentum label for each line and the graph rules are simplified accordingly.

Finally, we consider the application to a system with periodic inhomogeneity. For such a system the n -particle distribution function (23) is expected to remain unchanged under the translation \mathbf{R} of *all* particle coordinates, where \mathbf{R} is any lattice vector of the underlying Bravais lattice.⁸ This says in particular

$$p_1(\mathbf{r} + \mathbf{R}) = p_1(\mathbf{r}) \quad (61)$$

and

$$f_n(\mathbf{r}_1 + \mathbf{R}, \dots, \mathbf{r}_n + \mathbf{R}) = f_n(\mathbf{r}_1, \dots, \mathbf{r}_n). \quad (62)$$

It then follows from Eqs. (25) and (37) that

$$\pi(\mathbf{k}) = M \delta_{\mathbf{k}\mathbf{r}}(\mathbf{k}, \mathbf{G}) \tau(\mathbf{G}) \quad (63)$$

and

$$\theta(\mathbf{K}_1, \mathbf{K}_2) = M \delta_{\mathbf{K}\mathbf{r}}(\mathbf{K}_1 + \mathbf{K}_2, \mathbf{G}) \sigma(\mathbf{K}_1, \mathbf{K}_2), \quad (64)$$

where

$$\tau(\mathbf{G}) = \int_{\text{unit cell}} d\mathbf{r} p_1(\mathbf{r}) \exp(i\mathbf{G} \cdot \mathbf{r}), \quad (65)$$

and

$$\begin{aligned} \sigma(\mathbf{K}_1, \mathbf{K}_2) = & \int_{\text{unit cell}} d\mathbf{r}_1 \int d\mathbf{r}_2 f_2(\mathbf{r}_1, \mathbf{r}_2) \\ & \times \exp[-i(\mathbf{K}_1 \cdot \mathbf{r}_1 + \mathbf{K}_2 \cdot \mathbf{r}_2)]. \end{aligned} \quad (66)$$

In Eqs. (63) and (64), M is the number of unit cells of the periodic lattice, and \mathbf{G} is a reciprocal lattice vector satisfying

$$\exp(i\mathbf{G} \cdot \mathbf{R}) = 1. \quad (67)$$

Similarly, Eqs. (62), (26), and (28) imply that

$$U_n(\mathbf{k}_1, \dots, \mathbf{k}_n) = M \delta_{\mathbf{K}\mathbf{r}}(\mathbf{k}_1 + \dots + \mathbf{k}_n, \mathbf{G}) u_n, \quad n \geq 2, \quad (68)$$

where $u_n = O(1)$. Note that Eq. (68) is an exact result valid for any system satisfying Eq. (62).

V. CONCLUSION

We have evaluated in a closed form the multiple density correlation function I_n for a nonuniform system. The exact expression of I_n is given in Eqs. (27) and (28) in terms of the cluster integrals U_n . In Sec. III we generalized the convolution approximation for the n -particle distribution function to nonuniform systems, and used this approximation to evaluate U_n . This leads to the closed form expression (51) for U_n . Explicit expressions for $n=2, 3, 4$ are given in (53)–(55). Finally in Sec. V the formulation is specialized to specific systems including the case of a periodic inhomogeneity.

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⁸Equation (61) may be proved rigorously for a many-particle system in an external periodic potential. Let $T_{\mathbf{R}}$ be a translation operator which displaces *all* particle coordinates by \mathbf{R} . Since $T_{\mathbf{R}}$ commutes with the Hamiltonian, H , the wavefunction ψ can be chosen to be the simultaneous eigenfunction of $T_{\mathbf{R}}$ and H . Further, since $T_{\mathbf{R}} T_{\mathbf{R}'} = T_{\mathbf{R}+\mathbf{R}'}$, the eigenvalues of $T_{\mathbf{R}}$ are necessarily of the form $e^{i\mathbf{k}\cdot\mathbf{R}}$, or $T_{\mathbf{R}}\psi = e^{i\mathbf{k}\cdot\mathbf{R}}\psi$. The numbers \mathbf{k} are determined by the usual Born-von Karman boundary condition and are real. It follows then that $|T_{\mathbf{R}}\psi|^2 = |\psi|^2$ and, consequently, $T_{\mathbf{R}}p_n = p_n$.