Variational problem in Jastrow theory

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The ground-state wave function of an infinite system of fermions is approximated by the state-independent Jastrow ansatz. In order to optimize the pair correlation function, the Euler-Lagrange equations of the variational problem for the energy expectation value are derived. The short- and long-range behaviors of the optimum pair correlation function are discussed. Application of graphical techniques and use of rigorous results on the connection between the slope of the static structure function as $k \to 0+$ and long-range Jastrow correlations allow one to prove that the optimum pair correlation function behaves like $1 + O(r^{-2})$ as $r \to \infty$. A connection is derived between the weight of the long-range correlations and the Landau parameters. As simple examples the limit of Bose statistics and the electron-gas problem are considered. The consequences of these investigations on numerical calculations and their relation to alternative expansion methods are investigated.

I. INTRODUCTION

Jastrow theory has turned out to be a powerful tool for the computation of the ground-state properties of many-body quantum systems. Application of Jastrow theory to the Bose system ^{4}He [1,2] and the so-called homework problem[3] have yielded convincing results and hopefully even allow the prediction of a phase transition.[4,5]

The current interest in a detailed and quantitative description of neutron-star matter makes it desirable to achieve an elaborate state of the theory of Fermi systems which is comparable with that of Bose systems. As long as we do not want to go beyond Jastrow theory (by introduction of n-body ($n = 3, 4, \ldots$) correlations[6] or by use of nonorthogonal perturbation theory[7]), the requirements of such an elaboration can be focused in two steps.

(a) For a given Jastrow ansatz

$$\psi = F\Phi, \quad F \equiv \prod_{i<j}^{A} f(r_{ij}), \tag{1}$$

for the wave function (where the model wave function Φ is taken to be the ground-state function of a system of A independent fermions) we need a method to calculate physical quantities in which we are interested, i.e., first the energy expectation value

$$E = \langle\psi|H|\psi\rangle / \langle\psi|\psi\rangle, \tag{2}$$

but also the radial distribution function, the static structure function, and transport coefficients. In a first generation of work aiming at this point, cluster-expansion techniques have been established in close analogy to the cluster expansions of classical statistical mechanics.[8-10] A second generation of work carries out partial summations of infinite series of cluster contributions, which have a well-tested analogue in classical statistical mechanics and in the theory of Bose fluids.[11-13] Two of these methods, the first of which retains order by order special features of the Fermi system, take Fermi statistics systematically into account.[12,13] This has recently been extended[14] to a systematic method for obtaining the radial distribution function and the liquid structure function. It has been demonstrated to be well suited for the incorporation of long-range correlations and the study of the liquid structure function in the regime of low momenta. It will be shown below to be most appropriate for further investigations.

(b) Having found in step (a) a reliable approximation for the required physical quantities with respect to some *given* test wave function (1), we must now find a way to determine the *optimum* pair correlation function $f(r)$ in the sense that it minimizes the energy expectation value (2). This problem, which is the subject of the present paper, throws light on a number of difficulties which have up to now not been solved in a satisfactory way.

We consider the energy expectation value (2) with respect to the correlated wave function (1). For simplicity we assume the Hamiltonian to be of the form

$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} v(r_{ij}), \tag{3}$$

with a *state-independent* central potential $v(r)$. Our system is assumed to contain A fermions in a volume Ω with the number density $\rho = A/\Omega = \nu k_F^3/6\pi^2$, where ν is the degree of degeneracy of the single-particle states and k_F is the Fermi wave number.

Assuming that the Hamiltonian is bounded below, the variational problem

$$\delta E[f]/\delta f = 0 \tag{4}$$

has a solution which gives an upper bound to the ground-state energy. For practical reasons solving the full variational problem (4) is impossible and one is therefore forced to use approximations for $E[f]$ which generally arise from a cluster expansion. (Here we neglect the possibility of Monte Carlo calculations[2,15] in combination with a Feenberg expansion,[16] since the *optimum* Bose correlation function may be a *good* correlation function for Fermi systems, but will probably *not* be the *best* one.) The cluster-expansion techniques available up to now have the disadvantage that they break down for sufficiently long-ranged pair correlation functions $f(r)$ if they are truncated after a finite order. It is easily shown that for this reason the truncated expansion for the energy is generally no longer bounded below, forbidding the optimization of $f(r)$ by means of a free variation.[17]

To overcome this difficulty, subconditions on the pair correlation function have been introduced in order to keep $f(r)$ short ranged, i.e., to keep the "smallness parameter"

$$\xi \equiv \rho \int [f^2(\vec{r}) - 1]\, d^3r$$

finite.[18-21] Such a procedure is reasonable, since it can be assumed that the main contribution to the energy expectation value arises from the short-range correlations in the system, and it is necessary as long as no method is available to incorporate pair correlations which violate the condition $|\xi| < \infty$. The method of enforcing a sufficiently fast "healing" of $f(r)$ (i.e., approach to unity) is, however, to a certain extent arbitrary; the value of ξ (or some related quantity[17]) cannot, for example, be fixed from first principles, but must be estimated by convergence arguments. This freedom in the type of subconditions used therefore results in an uncertainty in the numerical values for the physical quantities to be computed which is apparently not too large for the ground-state energy, but which can be enormous for example for the compressibility.

Recent investigations of the Iwamoto-Yamada (IY) expansion[8,9] have uncovered a special feature of the Fermi system[12]: By combination of finite sets of cluster contributions it can be proven that all divergent portions cancel for correlation functions with an asymptotic behavior such as $f^2(r) - 1 \sim r^{-2}$. Furthermore, it has been shown that an r^{-2} healing of $f(r)$ is necessary in order to affect the slope of the static structure function in the region of small momenta.[14] Experimental results on ^{3}He [22,23] make it therefore most likely that long-range correlations are necessary to give a satisfactory description of Fermi fluids. It is the aim of this paper to consider the variational problem (4) and show that the *optimum* pair correlation function is in fact long ranged and of the r^{-2} type.

Because of the unboundedness of the energy expectation value in a truncated expansion we are not allowed to start our considerations with such an approximation, but are rather forced to consider the full variational problem (4) and try to find features of the *optimum* pair correlation function. These can be used to restrict the class of test functions in a numerical calculation with a *truncated* expansion for the energy.

In order to do this we start in Sec. II by giving a number of useful definitions required for the further considerations. Section III is devoted to the derivation of the Euler-Lagrange equation and the study of the short- and long-range behavior of the optimum pair correlation function. We will see that the optimum $f(r)$ has an r^{-2} healing which ensures us that the state of Jastrow theory achieved in preceding publications is sufficient to use the optimum pair correlation function.

Section IV gives the connection between the asymptotic term of $f^2(r) - 1$ derived in Sec. III to quantities to be obtained in a cluster expansion. To this aim we briefly outline the graphical representation of the IY expansion. In order to obtain general results we strictly follow the concept of reducing all quantities of interest to expressions of the highest possible connectivity. We will give a connection between the weight of the long-range correlation, the slope of the static structure function for small momenta, and the Landau parameters.

Although we are mainly interested in the study of Fermi systems, we can consider the corresponding Bose system by the simplification $\Phi = 1$. Thus we are able to compare results for the *optimum* Jastrow function derived from the variational problem with features of the *true* ground-state wave function of the Bose system. We will see in Sec. V that the asymptotic behavior of the optimum Jastrow function coincides qualitatively, but not quantitatively with the long-range part of the wave function of the Bose system as given by Feenberg.[16]

II. GENERALIZED DISTRIBUTION FUNCTIONS

In this section we strictly follow the methods invented by Feenberg[16] in order to obtain a compact representation of all quantities of interest, modifying some definitions to make the description more appropriate for Fermi systems.

From the identity

$$\Phi^* F\Delta_i F\Phi + \text{c.c.} = \Phi^* F^2 \Delta_i \Phi + \text{c.c.} + 2[\nabla_i(|\phi|^2 F\nabla_i F) - |\Phi|^2|\nabla_i F|^2], \tag{5}$$

which holds for any (not necessarily Jastrow) *real local* correlation operator F, we obtain for the energy expectation value

$$E = E_0 + \int |\psi|^2 V^* dr_1 \cdots dr_A \Big/ \int |\psi|^2 dr_1 \cdots dr_A, \tag{6}$$

with

$$V^* = \sum_i \left(\frac{\hbar^2}{2m}\right)|\nabla_i \ln F|^2 + \sum_{i<j} v(r_{ij}), \tag{7}$$

E_0 being the kinetic energy of a gas of free fermions. (In the definition of V^* we deviate from that given in Ref. 16.) In the case of a Jastrow correlation operator (1) the quantity V^* reduces to a sum of effective two- and three-body potentials:

$$V^* = \frac{1}{2}\sum_{i\neq j} w_2(i,j) + \frac{1}{2}\sum_{i\neq j\neq k} w_3(i;j,k), \tag{8}$$

with

$$w_2(i,j) \equiv v(r_{ij}) + (\hbar^2/m)|\nabla_i \ln f(r_{ij})|^2, \tag{9a}$$

$$w_3(i;j,k) \equiv (\hbar^2/m)\nabla_i \ln f(r_{ij}) \cdot \nabla_i \ln f(r_{ik}). \tag{9b}$$

(The symmetrization of $w_3(i;j,k)$ is possible and generally performed, but is not useful for our purpose.) We are now ready to introduce the *generalized normalization integral*

$$I(\beta) \equiv \int d^3r_1 \cdots d^3r_A |\psi|^2 e^{\beta V^*} \tag{10}$$

and the *generating function*

$$G(\beta) \equiv \ln I(\beta), \tag{11}$$

from which we obtain the energy expectation value by means of

$$E - E_0 = \frac{\partial}{\partial\beta} \ln I(\beta)\Big|_{\beta=0} = \frac{\partial}{\partial\beta} G(\beta)\Big|_{\beta=0} \tag{12}$$

and the squared norm of the wave function

$$\langle\psi|\psi\rangle = I(0). \tag{13}$$

The obvious decomposition of $E - E_0$ into

$$E - E_0 = E_{[2]} + E_{[3]}, \tag{14a}$$

with

$$E_{[2]} \equiv \frac{1}{2I(0)} \int d^3r_1 \cdots d^3r_A |\psi|^2 \sum_{i\neq j} w_2(r_{ij}), \tag{14b}$$

$$E_{[3]} \equiv \frac{1}{2I(0)} \int d^3r_1 \cdots d^3r_A |\psi|^2 \sum_{i\neq j\neq k} w_3(i;j,k), \tag{14c}$$

will be useful later.

Starting with the generalized normalization integral $I(\beta)$ we define generalized distribution functions

$$p^{(n)}(\vec{r}_1, \cdots, \vec{r}_n; \beta) \equiv \frac{A!}{(A-n)!} I(\beta)^{-1} \times \int d^3r_{n+1} \cdots d^3r_A |\psi|^2 e^{\beta V^*}, \tag{15}$$

which reduce for $\beta = 0$ to the familiar distribution functions. They obey the sequential relations

$$(A-n+1)p^{(n-1)}(\vec{r}_1 \cdots \vec{r}_{n-1}; \beta) = \int d^3r_n p^{(n)}(\vec{r}_1 \cdots \vec{r}_n; \beta). \tag{16}$$

In the special case $n = 2$ we define the *generalized radial distribution function*

$$g(r_{12}; \beta) \equiv \rho^{-2} p^{(2)}(\vec{r}_1, \vec{r}_2; \beta) \tag{17}$$

and the *generalized liquid-structure function*

$$S(k;\beta) \equiv 1 + \rho \int [g(r;\beta) - g(\infty;\beta)] e^{i\vec{k}\cdot\vec{r}}\, d^3r, \tag{18}$$

reducing for $\beta = 0$ to the familiar radial distribution function $g(r)$ and the liquid-structure function $S(k)$, respectively. For brevity we write

$$p^{(n)}(\vec{r}_1 \cdots \vec{r}_n) \equiv p^{(n)}(\vec{r}_1 \cdots \vec{r}_n; 0), \quad p^{(n)\prime}(\vec{r}_1 \cdots \vec{r}_n) \equiv \frac{\partial}{\partial\beta} p^{(n)}(\vec{r}_1 \cdots \vec{r}_n; \beta)|_{\beta=0}; \tag{19a}$$

$$S(k) \equiv S(k;0), \quad S'(k) \equiv \frac{\partial}{\partial\beta} S(k;\beta)\Big|_{\beta=0}, \tag{19b}$$

$$g(r) \equiv g(r;0), \quad g'(r) \equiv \frac{\partial}{\partial\beta} g(r;\beta)_{\beta=0}. \tag{19c}$$

The low-momentum behavior of the liquid-structure function $S(k)$ [which has been measured by x-ray scattering in ^{3}He (Refs. 22 and 23)] and the quantity $S'(k)$ will turn out to be of crucial importance for the discussion of the long-range behavior of the optimum pair correlation function.

Throughout this section we have assumed that all spin (and eventually isospin) summations have been performed.

III. VARIATIONAL PROBLEM

From the energy expectation value (2) we obtain by a straightforward variation with respect to $f(r)$ the Euler equation for the optimum pair correlation function $f^0(r)$. Using the definitions of Sec. II, we can write it in the form

$$\frac{\hbar^2}{m}\nabla_1\left(\frac{\nabla_1 f^0(r_{12})}{f^0(r_{12})}\,p^{(2)}(r_{12})+\int d^3r_3\frac{\nabla_1 f^0(r_{13})}{f^0(r_{13})}\,p^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3)\right)=p^{(2)\prime}(r_{12})\,. \tag{20}$$

(We have dropped the functional argument $f^0(r)$ from $p^{(2)}$, $p^{(3)}$, and $p^{(2)\prime}$.) This equation has been obtained by Lee and Broyles,[24] with the explicit representation

$$\begin{aligned}p^{(2)\prime}(r_{12})=&\,p^{(2)}(r_{12})w_2(r_{12})+\int d^3r_3 p^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3)[w_2(r_{13})+w_2(r_{23})]\\&+\frac{1}{2}\int d^3r_3\,d^3r_4[p^{(4)}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4)-p^{(2)}(r_{12})p^{(2)}(r_{34})]w_2(r_{34})\\&+\int d^3r_3 p^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3)[w_3(\vec{r}_1;\vec{r}_2,\vec{r}_3)+\text{c.p.}]+\int d^3r_3\,d^3r_4 p^{(4)}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4)[w_3(\vec{r}_1;\vec{r}_3,\vec{r}_4)+\text{c.p.}]\\&+\frac{1}{2}\int d^3r_3\,d^3r_4\,d^3r_5[p^{(5)}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4,\vec{r}_5)-p^{(2)}(r_{12})p^{(3)}(\vec{r}_3,\vec{r}_4,\vec{r}_5)]w_3(\vec{r}_3;\vec{r}_4,\vec{r}_5).\end{aligned} \tag{21}$$

The latter representation (of $p'(r)$) enables us to study the *short-range* behavior of the optimum pair correlation function: We observe that all the distribution functions $p^{(n)}$ occurring in Eqs. (20) and (21) have a common factor $f^2(r_{12})$ to cancel an apparent divergence of $v(r)$ and $\nabla f(r)/f(r)$ for $r\to 0$ or $r\to r_c$ where r_c is an assumed hard-core radius. Dividing Eq. (21) by this factor, we can collect all the remaining divergent contributions. They are contained in the first and fourth terms of the right-hand side of Eq. (21). We end up rewriting Eq. (20) in the form

$$(\hbar^2/m)\nabla[\nabla f^0(r)\,\hat{g}(r)]=f^0(r)[\hat{g}(r)v(r)+H(r)], \tag{22}$$

where $\hat{g}(r)\equiv g(r)/f^2(r)$ and $H(r)$ are *bounded* functions and $\hat{g}(r)$ does not in general vanish for vanishing $f(r)$. Clearly, Eq. (22) reduces to the radial Schrödinger equation for $r\to 0+$. Since Eq. (22) is only a rewriting of the Euler-Lagrange equation (20), it can be used with a reasonable ansatz for $\hat{g}(r)$ (in the lowest order it is the radial distribution function of a system of *independent* fermions) and $H(r)$ to determine the shape of $f^0(r)$ in the interaction-dominated region.[17,25] If we want to impose a subcondition of $f(r)$ in order to optimize only the short-range behavior, and introduce this subcondition to our variational problem by means of a Lagrangian multiplier, we should make sure that the structure of Eq. (22) is not destroyed. For example, it turns out that the condition

$$\kappa\equiv\rho\int[f(r)-1]^2\,d^3r<\infty, \tag{23}$$

originally suggested by Jastrow,[26] hurts the short-range behavior of $f(r)$ as indicated by Eq. (22), whereas Pandharipande's[19] generalization of the separation method[27] does not.

Returning to the main point of our considerations, the determination of the long-range behavior of $f^0(r)$, we again start from the Euler equation as given in Eq. (20). From the fact that the left-hand side of Eq. (20) is a gradient we conclude that the right-hand side vanishes asymptotically (and *does not* tend to a constant of order A^{-1}, as could be expected), yielding the relation

$$S'(0)=\rho^{-1}\int[p^{(2)\prime}(r)-p^{(2)\prime}(\infty)]\,d^3r=0 \tag{24}$$

as a first property of the optimum pair correlation function. However, as we shall see below, this relation is fulfilled by *any* pair correlation function in a Fermi system.

To proceed further we assume that the potential $v(r)$ is well behaved everywhere in order to guarantee that the Fourier transforms of all quantities exist. We stress, however, that this assumption is made only to make the calculations more transparent and to allow us to work with the familiar quantities introduced in Sec. II. The final results do *not* depend on our assumption. Thus we could, for example, cut off an infinite repulsive part of the potential at a certain level V_0, and take the limit $V_0\to\infty$ at the end of the calculation.

The discussion of the long-range behavior of the solution of the Euler equation (20) is most efficiently performed in Fourier space. We define

$$f^0(r)\equiv e^{u(r)/2} \tag{25}$$

and obtain, Fourier transforming Eq. (20),

$$(\hbar^2/2m)[-k^2u(k)S(k)+\tilde{D}(k)]=\rho^{-1}S'(k), \tag{26}$$

where the quantity $\tilde{D}(k)$ is the Fourier transform of

$$\begin{aligned}D(r_{12})=&\,\rho^{-2}\nabla\cdot(\nabla u(r_{12})[p^{(2)}(r_{12})-\rho^2]\\&+\int d^3r_3\nabla u(r_{13})[p^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3)-\rho p^{(2)}(r_{23})]).\end{aligned} \tag{27}$$

The important relation

$$k^{-2}D(k) \to 0 \quad (k \to 0+) \tag{28}$$

is easily proven to be a consequence of the sequential relations (16).

At this stage of our theory more information is required on the behavior of $S(k)$ and $S'(k)$ in the region of low momenta. This information can, for example, be provided by assumptions on the small-k behavior of $S(k)$ (one would assume a linear slope at least for the *optimum* Jastrow wave function) together with a reasonable ansatz for $S'(k)$.[28] However, a careful study of the cluster expansion has provided us with more information on $S(k)$ and $S'(k)$, which will be derived in Sec. IV. Our results are

$$S'(k) = S^2(k)B(k), \tag{29}$$

the function $B(k)$ being well behaved for short-ranged potentials, and

$$S(k) \sim k \quad (k \to 0+) \tag{30}$$

for *any* pair correlation function in the case of Fermi statistics. We therefore obtain, dividing Eq. (26) by $S^2(k)$,

$$\frac{\hbar^2\rho}{2m} \lim_{K\to 0+}\left(\frac{k^2u(k)}{S(k)}\right) = -\lim_{K\to 0+}\left(\frac{S'(k)}{S^2(k)}\right), \tag{31}$$

which yields $u(k) \sim \beta/k$ $(k \to 0+)$ corresponding to $u(r) \sim \beta/2\pi^2 r^2$ $(r \to \infty)$. Thus we have to be aware that we may obtain an r^{-2} behavior of the optimum pair correlation function. A similar result has been obtained for Bose systems: The *true* ground-state wave function contains long-range correlations (LRC's) of Jastrow type

$$u_{\mathrm{LRC}}^{\mathrm{Bose}}(r) \sim -mc/\pi^2\hbar\rho r^2, \quad (r \to \infty), \tag{32}$$

where c is the velocity of sound. We will see, however, that the optimization of the Jastrow ansatz yields for constant c a value which is slightly different from $(dp/md\rho)^{1/2}$. Nevertheless, the consideration of the variational problem and the comparison with rigorous results for the Bose system give strong arguments for the existence of long-range correlations in Fermi systems, although a direct physical interpretation is not yet obvious.

An equation of type (26) has been obtained by Pokrant and Stevens,[28] using the convolution approximation[29] for the higher distribution functions, in which case $S'(k) \sim S^2(k)$ $(k \to 0+)$ for short-ranged potentials and correlations such that $|r^2u(r)| < \infty$ $(r \to \infty)$. Application of graphical techniques allows one to prove that the same features are present in an *exact* treatment and shows the results of Pokrant and Stevens to be rigorous. The proof of this is the subject of Sec. IV.

IV. DIAGRAMMATIC METHODS

Having obtained a general formula governing the asymptotic behavior of the optimum pair correlation function, we now turn to an analysis of the quantities $S(k)$ and $S'(k)$ with the aim of computing the right-hand side of Eq. (31). To this end we start with a cluster expansion for the generating function $G(\beta)$ at $\beta = 0$. The rules governing the expansion can be expressed very effectively in a diagrammatic way,[12] originating from the Yvon-Mayer technique for classical systems and generalized by Gaudin *et al.*[30] for Fermi fluids. A systematic analysis of the expansion has been given elsewhere,[12] so we can restrict ourselves to surveying the graphical elements and the rules governing the expansion.

The basic elements of any diagram are (i) "internal" and "external" points (solid and open dots), (ii) "correlation lines" (dashed lines), and (iii) oriented "exchange lines" (oriented solid lines).

(i) An internal and an external point label the coordinates $\vec{r}_i$ of the ith particle. An internal point, furthermore, indicates a factor ρ and integration over the coordinate space of the particle involved.

(ii) A correlation line connecting the points $\vec{r}_i$ and $\vec{r}_j$ represents a correlation factor

$$\eta(|\vec{r}_i - \vec{r}_j|) = f^2(|\vec{r}_i - \vec{r}_j|) - 1.$$

(iii) An exchange line represents the exchange factor

$$l(k_F|\vec{r}_i - \vec{r}_j|) \quad [l(x) \equiv 3x^{-3}(\sin x - x\cos x)].$$

Typical diagrams are given in Figs. 1 and 2.

The general rules which determine the graphical construction are as follows:

(1) The cluster expansion for the generating function is the sum of all biconnected (or "irreducible") diagrams built from the graphical elements given above.

(2) Each point of a diagram is joined by at least one correlation line.

(3) Each point of a diagram is joined by at most one incoming (and one outgoing) exchange line. The exchange lines form closed loops, each loop connecting p points of the diagrams, contributes a factor $(-\nu)^{1-p}$, defining the sign of the diagram.

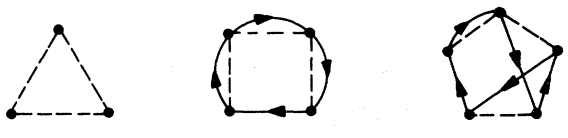

FIG. 1. Three diagrams without external points occurring in the graphical representation of the cluster expansion of $G(0)$.

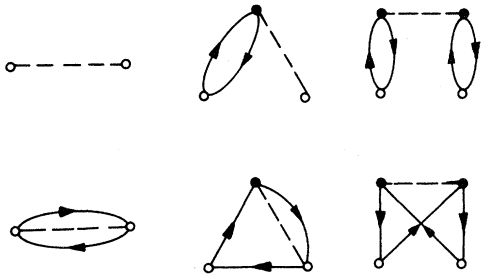

FIG. 2. Diagrams with two external points. They are all contributions to $g(r)$ with one correlation line. The three diagrams in the second line form all contributions to $L(r)$ with one correlation factor.

(4) The weight of each diagram with n points is given by its topological multiplicity divided by $n!$.

There is no need for the introduction of further graphical elements representing certain combinations of the lines defined here. We would end up only with more complicated rules governing the expansion and less transparency in our further considerations.

Attention should be paid to the occurrence of "equivalent" diagrams, i.e., diagrams with *different* topological structure which have the same value because of momentum conservation in the uniform extended medium. An example of equivalent diagrams is given in Fig. 3, and a general discussion may be found in Ref. 17 (see also Refs. 10 and 12). We obtain the final—but not always useful—graphical representation of $G(0)$ by collecting all equivalent diagrams.

From the graphical representation of $G(0)$ we now construct the energy expectation value as follows:

(1) The contribution $E_{[2]}$ is obtained from $G(0)$ by replacing in turn every correlation line by a "two-body effective interaction" line, representing a function $f^2(r_{ij})w_2(r_{ij})$.

(2) The contribution $E_{[3]}$ is obtained from $G(0)$ by replacing in turn every *connected pair* of correlation lines $\eta(r_{ij})\eta(r_{ik})$ by a pair of "three-body effective interaction" lines $f^2(r_{ij})f^2(r_{ik})w_3(\vec{r}_i;\vec{r}_j,\vec{r}_k)$ *before* collecting the equivalent diagrams.

From $E_{[2]}$ we obtain by comparison with

$$E_{[2]}=\frac{\rho^2}{2}\int d^3r_1\,d^3r_2 g(\vec{r}_{12})w_2(\vec{r}_{12}) \tag{33}$$

the radial distribution function $g(r)$. It is shown

FIG. 3. Simplest example of equivalent diagrams.

to be the sum of all irreducible diagrams with two external points ("irreducible 1-2 diagrams") which are permitted by the rules given above.[10]

The method of obtaining compact expressions for the radial distribution function has been described elsewhere;[12,14] thus we can restrict ourselves to giving the necessary definitions and the main results. For the definitions of graph theory we refer to Ref. 31. It is useful to define the following quantities:

$g_{DD}(r)$, the sum of all diagrams contributing to $g(r)$ with no exchange lines joined to the external points. (The trivial diagram representing the unity function is *not* included.)

$B(r)$, the sum of all *basic* diagrams with more than one correlation line and *no* exchange line joined to the external points.

$P(r)$, the same as $B(r)$, but with exchange lines joined to one selected external point (say $\vec{r}_1$), times a factor of ρ. By symmetry, $P(r)$ is $\frac{1}{2}$ of the sum of *all* basic diagrams with exchange lines joined to *any* of the external points.

$L(r)$, $\delta(\vec{r})$ plus ρ times the sum of all *basic* diagrams with exchange lines joined to *both* of the external points.

The sets of diagrams contributing to the functions $B(r)$, $P(r)$, and $L(r)$ are formed from the "renormalized correlation line" $g_{DD}(r)$ rather than from $\eta(r)$. The definition of *basic* diagrams has been extended in the sense that a basic diagram does *not* contain any proper 1-2 subdiagram, with *no* exchange lines joined to its external points except the single line $g_{DD}(r_{ij})$.

For the Fourier transforms $\tilde{B}(k)$, $\tilde{P}(k)$, and $\tilde{L}(k)$ the important relations can be shown (see Appendix):

$$|\tilde{B}(k)|<\infty \qquad (k\to 0+), \tag{34}$$

$$|k^{-1}\tilde{P}(k)|<\infty \qquad (k\to 0+), \tag{35}$$

$$|k^{-2}[\tilde{L}(k)-S_F(k)]|<\infty \qquad (k\to 0+). \tag{36}$$

Here, $S_F(k)$ is the liquid-structure function of a system of independent fermions.[15] It is the lowest-order contribution to the function $\tilde{L}(k)$.

With an analysis similar to that given in Ref. 31 (see also Ref. 32) for classical gases we obtained the generalized hypernetted-chain equations for Fermi systems[14]:

$$g_{DD}(r)=f^2(r)\exp[B(r)+N(r)]-1, \tag{37}$$

$$\tilde{N}(k)=\tilde{g}_{DD}(k)\{1-[1-\tilde{P}(k)]^2\}/[1+\rho\tilde{g}_{DD}(k)\tilde{L}(k)]. \tag{38}$$

Equation (38) may be used as a definition of the redundant function $N(r)$ [or $\tilde{N}(k)$]. For its diagrammatical interpretation see Ref. 31.

In terms of the quantities defined above the static structure function can be written

$$S(k) = \tilde{L}(k)[1 + \rho \tilde{g}_{DD}(k)\tilde{L}(k)]/[1 - \tilde{P}(k)]^2. \quad (39)$$

In the regime of low momenta the behavior of $S(k)$ depends crucially on the long-range part of $\eta(r)$. From Eqs. (34)–(39) we obtain

$$r^{-2}\eta(r) \to \beta/2\pi^2 \quad (r \to \infty)$$
$$\Rightarrow k^{-1}S(k) \to \alpha_F/(1 - \beta\rho\alpha_F) \quad (k \to 0+) \quad (40)$$

[$\alpha_F \equiv 3/4k_F$ is the slope of $S_F(k)$ as $k \to 0+$]. For correlations $r\eta(r) \to -\gamma$ $(r \to \infty)$, which might be appropriate for the investigation of the electron-gas problem, the only consistent solution of Eqs. (34)–(39) yields

$$r^2 g_{DD}(r) \to -1/2\pi^2\rho\alpha_F, \quad (r \to \infty), \quad (41)$$

$$k^{-2}S(k) \to 1/4\pi\rho\gamma, \quad (k \to 0+), \quad (42)$$

where Eq. (41) ensures that the quantities $B(r)$, $P(r)$, and $L(r)$, which have been defined to be diagrams in terms of the "renormalized" line $g_{DD}(r)$, exist.

The graphical representation of the function $g'(r)$ [and therefore $S'(k)$, which can be represented more easily] is obtained from the radial distribution function $g(r)$ by analogy with the derivation of the energy from the generating function $G(0)$. We must (1) drop all contributions to $g(r)$ which contain *no* correlation line, (2) replace in turn each correlation line by a two-body effective interaction line, and (3) replace (before collecting equivalent diagrams) each connected pair of correlation lines by a pair of effective three-body interaction lines.

Consequently, we can represent $g'(r)$ as a sum of nodal and non-nodal diagrams. In each diagram, only one non-nodal subdiagram containing effective (two- or three-body) interaction lines can occur, or two connected non-nodal subdiagrams, containing the effective three-body interaction lines $(\hbar^2/m)f(r_{ij})\nabla_i f(r_{ij}) \cdot \nabla_i f(r_{ik}) f(r_{ik})$, where $\vec{r}_j$ is a field point of one subdiagram, $\vec{r}_k$ of the other, and $\vec{r}_i$ the node between them.

We denote the sum of non-nodal subdiagrams of $g'(r)$, which contain effective two- (or a pair of effective three-) body interaction lines and exchange lines joined to none, one selected, and both of the external points, by $g'^N_{DD}(r)$, $g'^N_{DE}(r)$, and $g'^N_{EE}(r)$, respectively. Along the same lines as in the proof of Eqs. (34)–(36) we can show for the Fourier transforms of these functions $(k \to 0+)$

$$\tilde{g}'^N_{DD}(k) \to \gamma_{DD} < \infty,$$
$$k^{-1}\tilde{g}'^N_{DE}(k) \to \gamma_{DE} < \infty, \quad (43)$$
$$k^{-2}\tilde{g}'^N_{EE}(k) \to \gamma_{EE} < \infty.$$

The function $g'(r)$ is now obtained by summing all possible combinations of the quantities $g'^N_{DD}(r)$, $g'^N_{DE}(r)$, and $g'^N_{EE}(r)$ and the pairs of diagrams connected by $w_3(i;j,k)$ with the constituents of the radial distribution function. Suppressing technical details we obtain for the right-hand side of Eq. (31) (with $\gamma \equiv \gamma_{DD} + 2\alpha_F^{-1}\gamma_{DE} + \alpha_F^{-2}\gamma_{EE}$)

$$\lim_{k\to 0+}\left(\frac{S'(k)}{S^2(k)}\right) = \rho\gamma + \frac{\hbar^2\rho^2}{4m}\lim_{k\to 0+} k^2u^2(k). \quad (44)$$

A set of useful formulas for the computation of γ_{DD}, γ_{DE}, and γ_{EE} is given in the Appendix.

In combination with Eqs. (31) and (40) we find for the strength β of the long-range correlations an equation

$$\beta^2 - 2\beta/\rho\alpha_F = m\gamma/\hbar^2\rho \quad (45)$$

or, solving for the slope α of the static structure function as $k \to 0+$,

$$\alpha^{-2} = \alpha_F^{-2} + 4\rho\gamma m/\hbar^2. \quad (46)$$

In general, the quantity γ does not vanish. Equations (45) and (46) give us therefore, together with Eqs. (30), (40), and (43), a tool for the calculation of the long-range part of the optimum pair correlation function.

The physical interpretation of the slope α of $S(k)$ as $k \to 0+$ has been subject to several discussions.[33,34] An interesting relation to Landau theory can be established if we neglect the dependence of the *optimum* $f(r)$ on the quasiparticle distribution function: In this case, cluster expansions for the Landau parameters

$$F_l^s = \sum_n (\Delta F_l^s)_n \quad (47)$$

can be derived in analogy to the expansion for the energy expectation value. A direct comparison of the cluster contributions $(\Delta F_l^s)_n$ and the expansions for γ_{DD}, γ_{DE}, and γ_{EE} given in the Appendix yields

$$\gamma = \frac{2\hbar^2\pi^2}{\nu m^* k_F}\left(F_0^s - \frac{4F_1^s}{9} + \sum_l (-1)^l \beta_l^2 F_{2l}^s\right), \quad (48)$$

with

$$\beta_l \equiv (2l-2)!/[2^{2l-1}(l-1)!(l+1)!], \quad (49)$$

and therefore

$$\frac{\alpha}{\alpha_F} = \left[1 + \frac{3m}{4m^*}\left(F_0^s - \frac{4F_1^s}{9} + \sum_l (-1)^l \beta_l^2 F_{2l}^s\right)\right]^{-1/2} \quad (50)$$

A more detailed derivation of expressions for Landau parameters within our framework will be given elsewhere.

Using the experimental values $F_0^s = 10.8$, $F_1^s = 6.25$ given by Abel *et al.*[35] and neglecting all F_l^s for $l \geq 2$, we obtain from Eq. (50) $\alpha/\alpha_F = 0.582$, in excellent agreement with the result $\alpha/\alpha_F = 0.575$

given by Widom and Siegel, who obtained it by a completely different formula, but also by application of Landau theory. The agreement with the experimental value $\alpha/\alpha_F \approx 0.4$ is, however, not too satisfactory. The reason for the deviation may be the neglect of more complicated correlations by the simple Jastrow ansatz (1) [which apparently causes Eq. (50) to have a simple form] and the neglect of the dependence of $f(r)$ on the density.

V. DISCUSSION

To get a feeling for the importance of the density dependence of $f(r)$ and the limitations of the Jastrow ansatz (1) we consider the simple limit of Bose statistics. Here, it is known that the *true* ground-state wave function contains long-range correlations of Jastrow type[16] [see Eq. (32)]. Furthermore, the limit $\alpha = \lim_{k\to 0+} k^{-1}S(k)$ is known to be $\alpha = \hbar/2mc$.

Within our framework, we obtain a theory of the Bose system by dropping all contributions which contain exchange lines, or, equivalently, taking the limit $k_F \to 0$, $\nu \to \infty$, ρ fixed. The energy expectation value is now the sum of all irreducible diagrams with one effective two-body (or a pair of effective three-body) interaction lines. Classifying with respect to the *number of particles* involved, we can write the cluster expansion in the form

$$\frac{E}{A} = \sum_n \frac{(\Delta E)_n}{A} = \sum_n \rho^{n-1} e_n, \tag{51}$$

where $e_n \equiv (\Delta E)_n / \rho^{n-1} A$ depends on density *only* via the density dependence of the pair correlation function $f(r)$. The function $g'^N_{DD}(r)$, which is the only surviving contribution in Eq. (43), is now easily obtained from the energy expectation value: To obtain all *non-nodal* n-particle diagrams with two external points we have to make in all *irreducible* n-particle diagrams two points external. This can be done in $\frac{1}{2}n(n-1)$ ways. Fourier transforming and taking the limit $k \to 0+$, which is equivalent to integrating over coordinate space, leaves us with $n(n-1)/2\Omega$ times the original diagrams. We therefore obtain from Eq. (51)

$$\gamma_{DD} = \sum_{n\geq 2} \frac{n(n-1)}{2\rho} \frac{(\Delta E)_n}{A} = \sum_{n\geq 2} \frac{n(n-1)}{2} \rho^{n-2} e_n, \tag{52}$$

and therefore

$$\rho\gamma_{DD} = \frac{\partial}{\partial\rho}\rho^2 \frac{\partial}{\partial\rho}\frac{E}{A} \equiv mc^{*2}, \tag{53}$$

defining the quantity c^*, which has the dimension of a velocity. For the partial differentiation in Eq. (53) with respect to ρ we understand that $f(r)$ is kept fixed.

From Eq. (46) we now obtain in the limit of Bose statistics (i.e., $\alpha_F \to \infty$)

$$S(k) \sim \hbar k/2mc^* \quad (k \to 0+), \tag{54}$$

or, equivalently,

$$u(r) \sim -mc^*/\pi^2\hbar\rho r^2 \quad (r \to \infty). \tag{55}$$

The quantity c^* is immediately seen *not* to be the velocity of sound $c = (dp/md\rho)^{1/2}$. Recalling that we have optimized $f(r)$ for *any* density, i.e., that we have the conditions $\delta E/\delta f = 0$ *and* $(d/d\rho)\delta E/\delta f = 0$, we obtain

$$m(c^{*2} - c^2) = \Omega^{-1} \int d^3r_1\, d^3r_2 \frac{\delta^2 E}{\delta f^2}(\vec{r}_1, \vec{r}_2) \frac{df(r_1)}{d\rho}\frac{df(r_2)}{d\rho}, \tag{56}$$

i.e., c^* is larger than the velocity of sound under the weak assumptions that the Jastrow state is *stable* and that the *optimum* pair correlation function is density dependent. The latter holds, as we can see from Eq. (55), provided that the equation of state in the density region under consideration is *not* of the special form $p - p_0 \sim \rho^3$. We find that our simple Jastrow ansatz (1) for the wave function gives qualitative, but not quantitative, coincidence with rigorous results on the static structure function. Obviously, this is merely an effect of the simplicity of our ansatz (1). The difference $c^{*2} - c^2$ may, however, indicate a region where our approximation is reasonable and give a feeling for the density regimes where more complicated correlations become important. Furthermore, Eqs. (53) and (54) may give a consistency test for optimization procedures which have been developed for Bose systems[6,16] and appear to be easier to use for numerical calculations than the method presented here.

An iterative optimization procedure, which is similar to the paired-phonon analysis (PPA)[16] for Bose systems, unfortunately does not yet exist for Fermi fluids. The method presented here seems to be an attractive way to obtain an optimum $f(r)$ without running into the difficulty of the unboundedness of the energy expectation value or having to argue about subconditions which cannot be derived from first principles. The asymptotics of the correlation function are fixed by Eq. (45); its short-range structure may be optimized either by Eq. (22) or by a Ritz variational approach. The expansion (52) for Bose systems may give an estimate for the distinct contributions to the cluster expansion of γ. Because of the factors $\frac{1}{2}n(n-1)$ we have to take account of a considerably slower convergence of the series. In particular, truncating the

expansion (52) after the lowest-order contribution $(\Delta E)_2$, we obtain

$$\alpha_{(2)}^{-2} \approx \alpha_F^{-2} + 4m(\Delta E)_2/A\hbar^2. \tag{57}$$

For ^{3}He, $(\Delta E)_2/A$ is the leading contribution to the binding energy and should be negative in order to guarantee a sufficiently fast convergence of the expansion for the energy, which yields $\alpha > \alpha_F$. We see that the lowest correction to α is of the wrong sign and has to be overcompensated by the higher contributions. In view of the relatively bad convergence of the cluster expansion of γ, summations of infinite partial series are highly desirable. However, having adopted the scheme of incorporating exchange contributions properly, these summations seem to be purely technical. Because of the close relation between γ and the Landau parameters the same argument holds for the latter, too: Computations of transport coefficients in the lowest order of our cluster expansion may be completely misleading.[36]

We emphasize that our result on the asymptotics of the optimum pair correlation function depends essentially on the features $S(0+) = S'(0+) = 0$. These features can be shown to be present order by order in a cluster expansion for $g(r)$ or $g'(r)$, if we classify with respect to the number of correlation lines involved[17] [power-series (PS) classification[10]]. However, a factor $f^2(r) = \eta(r) + 1$ is needed in the radial distribution function in order to cancel a strong repulsive part of the potential. *Any* approximation for the radial distribution function extracted [by use of Eq. (33)] from a *truncated* expansion for the energy will therefore not rigorously yield $S(0+) = 0$. Even in a reliable approximation for the energy expectation value, which is bounded below and allows therefore for a free variation with respect to the pair correlation function, we can not hope to determine the *optimum* $f(r)$ by means of a variation of the energy expectation value. We are, on the other hand, not forced to extract $S(k)$ via $g(r)$ from some approximation for the energy, but may rather use more suitable approximations (e.g., the PS expansion). We are therefore able to compute $\lim_{k\to 0+}[S'(k)/S(k)^2]$ order by order without any assumptions on the potential. An additional summation of the perturbation series, as suggested by Talman[37] (who arrived at our results in the lowest order of the PS expansion, but unfortunately does not give relations to physical quantities), seems therefore avoidable in our context.

The fact that after the generalized hypernetted-chain summation is performed our expansion is even applicable for r^{-1} correlations allows us to consideration the electron-gas problem. Here, the first of the equations (43) is no longer valid, and the lowest-order contribution to $g'^N_{DD}(r)$ if of the form

$$[\Delta g'^N_{DD}(r)]_2 = f^2(r)e^2/r + (\hbar^2/m)f'^2(r), \tag{58}$$

yielding

$$\frac{S'(k)}{S(k)^2} = \frac{4\pi\rho e^2}{k^2} + \frac{\hbar^2\rho^2}{4m}\, k^2 u^2(k) \quad (k \to 0+). \tag{59}$$

[In all higher-order contributions to $g'^N_{DD}(r)$, and in $g'^N_{DE}(r)$ and $g'^N_{EE}(r)$, the potential $v(r)$ is multiplied with functions which decrease sufficiently fast asymptotically.]

Now, Eqs. (31), (41), (42), and (59) give

$$u(r) = e^2/(2\hbar\omega_{pl}r) \quad (r \to \infty), \tag{60}$$

with $\omega_{pl} \equiv (4\pi e^2\rho/m)^{1/2}$ being the plasma frequency. We thus have reproduced the results obtained by Bohm and Pines[38] and those of several other approximation methods.[28]

The analysis presented in this paper gives not only a tool for the computation of the optimum pair correlation function in Fermi systems (and therefore of all physical quantities of interest), but also allows for a critical investigation of different cluster-expansion techniques from the point of view of their suitability in an optimization procedure.

A considerable amount of work has been done to renormalize the IY expansion in *momentum space*.[39-41] This type of renormalization yields an expansion which can be considered as an analog to the activity expansion of classical statistical mechanics[42]; it is also so far the only cluster-expansion technique for Fermi systems for which rigorous results on the convergence behavior have been derived.[43] Restricting ourselves to the Jastrow ansatz for the correlation function, this means that our expansion is no longer irreducible in *coordinate space*. Therefore this renormalization aims in just the opposite direction to what is experienced in classical statistical mechanics and in the theory of Bose systems, namely, that an expansion converges better with higher connectivity of the distinct contributions. In Fermi systems we even lose one more advantage of the irreducible expansion: There is no longer a cancellation of divergent portions in the case of long-range correlations. It is therefore impossible to use the optimum Jastrow function in this type of renormalized expansion. These arguments are supported by an extensive numerical study by Nitsch.[41]

The situation becomes less clear if we admit more complicated correlation operators.[39] Here, it is still open whether one should prefer an irreducibility in *momentum space* rather than in coordinate space. But even in this case the *un-*

renormalized IY expansion fulfills automatically *order by order* exact properties [as $g(r) \to 1 + O(\Omega^{-1})$ $(r \to \infty)$, and, after some reordering in analogy to the PS scheme, fulfills $S(0+, \beta) = 0$],[17] whereas the renormalized version does not.

Other approaches perform distinct summations of partial series in order to reduce all quantities to diagrams of higher connectivity in coordinate space. All these methods have originally been constructed to treat short-range correlations only.[11,13] In particular, in the method of Fantoni and Rosati[13] the possibility of incorporating long-range correlations has not been investigated. It would be interesting to see whether these alternative techniques—which might be of equal usefullness as long as only short-ranged pair correlations are considered—are also suitable for the full, unconstrained variational problem.

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APPENDIX: PROOF OF THE RELATIONS (34)–(36) AND (43)

The two proofs follow the same lines. The only difference is that the diagrams forming the sets $g'^N_{DD}(r)$, $g'^N_{DE}(r)$, and $g'^N_{EE}(r)$ contain effective interaction lines, whereas $B(r)$, $P(r)$, and $L(r)$ do not.

The evaluation of

$$\gamma_{DD} \equiv \lim_{k \to 0+} \tilde{g}'^N_{DD}(k)$$

is trivial. By definition we have

$$\gamma_{DD} = \int d^3r g'^N_{DD}(\vec{r}). \tag{A1}$$

For the computation of γ_{DE} we consider a diagram with exchange lines *and* at least one correlation (or interaction) line joined to one of the external points (say, $\vec{r}_1$). It can be written in the form

$$D_1(|\vec{r}_1 - \vec{r}_2|) = \int d^3r_3 G_{DE}(\vec{r}_1, \vec{r}_2, \vec{r}_3) l(k_F r_{13}). \tag{A2}$$

With the same weight the contribution

$$D_2(|\vec{r}_1 - \vec{r}_2|) = \frac{\rho}{\gamma} \int d^3r_3 \, d^3r_4 \, G_{DE}(\vec{r}_4, \vec{r}_2, \vec{r}_3) l(k_F r_{13}) l(k_F r_{14}) \tag{A3}$$

occurs in our expansion for $g'^N_{DE}(r)$, which has *no* correlation line joined to the external point $\vec{r}_1$. From the relation

$$\int d^3r' l(k_F|\vec{r} - \vec{r}'|) l(k_F r') = (\nu/\rho) l(k_F r), \tag{A4}$$

we obtain that the sum $\lim_{k \to 0+} [\tilde{D}_1(k) + \tilde{D}_2(k)]$ vanishes. The quantity of interest, $d/dk[\tilde{D}_1(k) + \tilde{D}_2(k)]|_{k=0+}$, is most efficiently computed introducing cylindrical coordinates in Fourier space. After some elementary manipulations we arrive at

$$\frac{d}{dk}[\tilde{D}_1(k) + \tilde{D}_2(k)]|_{k=0+} = \alpha_F \int d^3r_{12} \, d^3r_3 \, G_{DE}(\vec{r}_1, \vec{r}_2, \vec{r}_3) j_0(r_{13} k_F). \tag{A5}$$

The computation of γ_{EE} is similar: We start with a contribution to $g'^N_{EE}(r)$ with exchange lines *and* correlation lines joined to both of the external points. It can be written as the form

$$D_{11}(|\vec{r}_1 - \vec{r}_2|) = \int G_{EE}(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4) \times l(k_F r_{13}) l(k_F r_{24}) \, d^3r_3 \, d^3r_4 . \tag{A6}$$

With the same weight the contributions

$$D_{12}(|\vec{r}_1 - \vec{r}_2|) = -\frac{\rho}{\gamma} \int G_{EE}(\vec{r}_5, \vec{r}_2, \vec{r}_3, \vec{r}_4) l(k_F r_{15}) l(k_F r_{13}) l(k_F r_{24}) \, d^3r_3 \, d^3r_4 \, d^3r_5 ,$$

$$D_{21}(|\vec{r}_1 - \vec{r}_2|) = -\frac{\rho}{\gamma} \int G_{EE}(\vec{r}_1, \vec{r}_6, \vec{r}_3, \vec{r}_4) l(k_F r_{13}) l(k_F r_{24}) l(k_F r_{26}) \, d^3r_3 \, d^3r_4 \, d^3r_6 ,$$

$$D_{22}(|\vec{r}_1 - \vec{r}_2|) = \frac{\rho^2}{\nu^2} \int G_{EE}(\vec{r}_5, \vec{r}_6, \vec{r}_3, \vec{r}_4) l(k_F r_{15}) l(k_F r_{13}) l(k_F r_{24}) l(k_F r_{26}) \, d^3r_3 \, d^3r_4 \, d^3r_5 \, d^3r_6 \tag{A7}$$

occur in $g'^N_{EE}(r)$, which has no correlation line joined to $\vec{r}_1, \vec{r}_2$, or both, respectively. The computation of $\lim_{k \to 0+} k^{-2}[\tilde{D}_{11}(k) + \tilde{D}_{12}(k) + \tilde{D}_{21}(k) + \tilde{D}_{22}(k)]$ is again elementary and most efficiently performed introducing cylindrical coordinates in Fourier space. After some lengthy calculations one arrives at

$$\lim_{k\to 0+} k^{-2}[\tilde{D}_{11}(k)+\tilde{D}_{12}(k)+\tilde{D}_{21}(k)+\tilde{D}_{22}(k)]$$

$$=\alpha_F{}^2\sum_l(-1)^l(2l+1)b_l^2\int G_{EE}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4)j_l(r_{13}k_F)j_l(r_{24}k_F)P_l(\cos\measuredangle(r_{13},r_{24}))d^3r_{12}\,d^3r_3\,d^3r_4\,, \quad \text{(A8)}$$

with

$$b_l\equiv 2\int_0^1 xP_l(x)\,dx. \quad \text{(A9)}$$

The $P_l(x)$ are the Legendre polynomials. The coefficients b_l are found to be

$$b_0=\tfrac{1}{2},\quad b_1=\tfrac{1}{3},\qquad b_l=\begin{cases}(l-2)!/[2^l(\frac{1}{2}l-1)!(\frac{1}{2}l+1)!] & l \text{ even},\\ 0, & l \text{ odd},\end{cases} \quad \text{(A10)}$$

for $l\geq 2$.

The proof of the properties (34)–(36) is the essential step in proving by induction the existence of the power-series expansion for long-range correlations.

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