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Theory of inhomogeneous quantum systems. III. Variational wave functions for Fermi fluids

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We develop a general variational theory for inhomogeneous Fermi systems such as the electron gas in a metal surface, the surface of liquid ^{3}He, or simple models of heavy nuclei. The ground-state wave function is expressed in terms of two-body correlations, a one-body attenuation factor, and a model-system Slater determinant. Massive partial summations of cluster expansions are performed by means of Born-Green-Yvon and hypernetted-chain techniques. An optimal single-particle basis is generated by a generalized Hartree-Fock equation in which the two-body correlations screen the bare interparticle interaction. The optimization of the pair correlations leads to a state-averaged random-phase-approximation equation and a strictly microscopic determination of the particle-hole interaction.

I. INTRODUCTION

This paper is the third in a series of papers developing and applying a variational theory of inhomogeneous systems. The first two papers in this series (Refs. 1 and 2, hereafter called papers I and II) were devoted to the formulation of the variational theory of the ground state[1] and the collective excitations[2] in Bose systems and the numerical application of that theory to films of ^{4}He. We extend the theory here to Fermi systems. This project reveals a number of challenging problems. We emphasize our goal of designing a *consistent* and *practical* theoretical description of inhomogeneous Fermi systems.

The variational method for an interacting many-particle system starts with an explicit *ansatz* for the ground-state wave functions, usually of the Feenberg form,[3]

$$|\Psi_0\rangle = \exp\left[\tfrac{1}{2}\sum_i u_1(\mathbf{r}_i) + \tfrac{1}{2}\sum_{i<j} u_2(\mathbf{r}_i,\mathbf{r}_j) + \cdots\right] |\Phi_0\rangle/\mathcal{N}\ , \tag{1.1}$$

which is made unique by requiring that each of the $u_i(\mathbf{r}_1,\ldots,\mathbf{r}_i)$ satisfies the *cluster property.*[3] $|\Phi_0\rangle$ is the ground-state wave function of a suitably chosen model system which reflects the *statistics* and the *symmetries* of the physical system under consideration. $\mathcal{N}$ is the norm. We assume that the model system is described by a one-body Hamiltonian. Hence, in a Bose system, $|\Phi_0\rangle$ is the symmetrized product of the lowest eigenfunction of this one-body Hamiltonian. It may be absorbed, without loss of generality, in the one-body correlation factor $u_1(\mathbf{r})$. In an A-body Fermi system, $|\Phi_0\rangle$ is the Slater determinant of the A lowest eigenstates of that one-body Hamiltonian. In a sense, the one-body correlation factor $u_1(\mathbf{r})$ is also redundant; we will address this question below in much greater detail.

The n-body correlation factors $u_1(\mathbf{r})$, $u_2(\mathbf{r}_i,\mathbf{r}_j),\ldots$, are determined by minimization of the ground-state energy:

$$\frac{\delta\langle\Psi_0|H|\Psi_0\rangle}{\delta u_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)} = 0 \quad (n=1,2,\ldots)\ . \tag{1.2}$$

We develop in this work a general theoretical framework in which the variational theory of inhomogeneous Fermi systems can be formulated and applied numerically. The simplest consistent version of the theory is described in some detail. A discussion of the possible routes for a systematic application of the theory to various systems of physical interest will be given at the end of this paper when the formal parts of the theory are available.

It is worthwhile to reiterate an argument of I concerning a minimum criterion that a microscopic theory for an inhomogeneous system should fulfill. That is, such a theory should allow for an unambiguous prediction of whether a number A of particles within a given volume V fills this volume homogeneously, or only partly. The transition between the homogeneous and the inhomogeneous phases occurs when the density of particles is decreased. Below the saturation density there is normally a metastable regime in which the pressure of the homogeneous phase is negative, but the compressibility is still positive. If the density decreases even more, the compressibility goes to zero and the system becomes *locally* unstable against density fluctuations. A theory that covers both the homogeneous and the inhomogeneous phase should clearly exhibit such an instability of the homogeneous phase when its density is decreased. This requires, in the language of perturbation theory, the (approximate) self-consistent summation of ring and ladder diagrams.[4] The optimized Fermi-hypernetted-chain (FHNC) theory[5] is at present the only practically used microscopic theory for a

Fermi system which fulfills[6] this requirement.

Let us briefly review the connection between our theory and earlier microscopic approaches to the study of inhomogeneous Fermi systems. The present work is primarily designed for quantitative microscopic studies of the electron liquid in a metal surface and for the free surface of liquid ^{3}He. Our theory is closely related to the pioneering effort by Woo and collaborators,[7] who were the first to apply variational methods to inhomogeneous Fermi systems. We deviate from the approach developed by Woo in that we use the more common FHNC technique of cluster expansions and summations for Fermi systems and employ an explicit optimization procedure. Compared with perturbative microscopic approaches, our theory can be understood as a special implementation of the parquet-diagram theory[4] which sums self-consistently all ring and ladder diagrams.

The most popular alternative theory used for the study of metal surfaces is the density-functional theory.[8] The relation to that theory has to be studied in detail in the future; we anticipate that the variational approach can be understood as a microscopic derivation of the Kohn-Sham potential.

We give now an overview of the organization of this paper. The choice of the single-particle orbitals is quite straightforward in the Bose case, but it causes a number of problems in the Fermion case. Care is required to maintain the cluster property of the two-body correlation factor $u_2(\mathbf{r}_i,\mathbf{r}_j)$. We will address these questions in the next section, where we discuss the choice of the single-particle basis and the consequences of the one-body attenuation factor $u_1(\mathbf{r})$.

A systematic cluster expansion and summation method is introduced in Sec. III. As in earlier developments,[5,6] special attention is paid to the proper treatment of the Pauli principle in the intermediate states. This calls for specific and consistent truncation schemes in the cluster expansions of one- and two-body quantities. The developments of Secs. II and III were to some extent forecast by Ripka;[9] we will go beyond the formalism of that work in a number of aspects which are important for both understanding and implementing the theory. Section IV addresses the calculation of the energy expectation value and the optimal determination of the single-particle basis. An optimal choice of the single-particle basis leads to substantial simplifications.

Section V reviews the Fermi-hypernetted-chain theory and gives the simplest acceptable implementation of that theory for an inhomogeneous system. Consistency requirements between systematic approximations for one- and two-body quantities are discussed.

Section VI describes the determination of the two-body correlations via the variational principle (1.2). As in I, we formulate the theory in a random-phase-approximation (RPA) —like manner which emphasizes the intermediate- and long-ranged correlations and is adaptable to numerical optimization via the "paired-phonon analysis"[10] (PPA). The emphasis of intermediate- and long-ranged correlations is not so much dictated by our immediate goal of developing a theory of metal surfaces. Rather, the short-ranged correlations are in most cases quite well known from low-order methods, whereas the intermediate- and long-ranged correlations are usually difficult to estimate, and considerably affected by the inhomogeneity of the system. Hence, an optimization strategy which is especially efficient in that regime should be the method of choice. A discussion of the application of our theory to different physical systems—electron gas, terrestrial quantum fluids, and nuclear many-body systems is given in the concluding section.

II. SINGLE-PARTICLE ORBITALS

In the Fermi system under consideration here, the "noninteracting" model state $|\Phi_0\rangle$ [cf. Eq. (1.1)] is the determinant of a set of single-particle orbitals $\phi_i(j)\equiv\phi_i(\mathbf{r}_j)\chi(i)$, $i,j=1,\ldots,A$, i.e.,

$$|\Phi_0\rangle=\det|\phi_i(\mathbf{r}_j)\chi(i)| \ . \tag{2.1}$$

The $\chi(i)$ are the spin eigenfunctions. The spatial single-particle orbitals $\phi_i(\mathbf{r}_j)$ are usually generated by a one-body equation,

$$H_1[\phi_k]\phi_i(\mathbf{r}_j)=\epsilon_i\phi_i(\mathbf{r}_j) \ . \tag{2.2}$$

To be specific we may assume a Hartree or Hartree-Fock form, which allows $H_1[\phi_k]$ to be a functional of the single-particle orbitals. For the time being, no assumption is made on the method by which the single-particle states are generated; a unique procedure will later emerge from the variational principle (1.2). It is clear that all physical observables are independent of the single-particle basis in which we choose to generate the basis functions of the Hilbert space. In practice, however, one often works with expansions and approximations, and a suitable choice of the single-particle basis may well affect the structure of the expansion and the convergence rate of an approximation scheme. The same feature will appear in the variational theory developed in this paper.

To make this more explicit, let us now draw attention to the one-body attenuation factor $u_1(\mathbf{r})$ in the correlation function (1.1). This factor looks redundant; it may be absorbed by redefining the single-particle orbitals as

$$\phi_i(\mathbf{r})\rightarrow\exp[\tfrac{1}{2}u_1(\mathbf{r})]\phi_i(\mathbf{r}) \ . \tag{2.3}$$

However, this redefinition destroys the orthogonality of the "new" single-particle states. On the other hand, the inclusion of the one-body attenuation factor is generally necessary[1] in order to guarantee that the solution of the two-body Euler equation,

$$\frac{\delta\langle\Psi_0|H|\Psi_0\rangle}{\delta u_2(\mathbf{r}_1,\mathbf{r}_2)}=0 \ , \tag{2.4}$$

satisfies the cluster property,

$$u_2(\mathbf{r}_1,\mathbf{r}_2)\rightarrow 0 \ \text{ as } \ |\mathbf{r}_1-\mathbf{r}_2|\rightarrow\infty \ . \tag{2.5}$$

One of the main results of this paper is the explicit construction of an "optimal" single-particle basis which minimizes the energy-expectation value while guaranteeing the cluster property (2.5). Constructing this basis requires the development of cluster expansions which do include one-body factors in the Feenberg function.

Let us consider the distribution functions generated by the simplified correlated wave function,

$$|\Psi_0^{(1)}\rangle=\exp\left[\tfrac{1}{2}\sum_i u_1(\mathbf{r}_i)\right]|\Phi_0\rangle/\mathcal{N}\ , \tag{2.6}$$

i.e., the correlated wave function (1.1) without the two-body correlations. It is convenient to start by defining a generating functional,

$$G_F\equiv\ln\left\langle\Phi_0\left|\exp\left[\sum_i u_1(\mathbf{r}_i)\right]\right|\Phi_0\right\rangle\ , \tag{2.7}$$

and derive from this functional one- and two-body densities by functional differentiation:

$$\frac{\delta G_F}{\delta u_1(\mathbf{r})}=\rho_1^F(u_1\,|\,\mathbf{r})\ , \tag{2.8}$$

$$\frac{\delta^2 G_F}{\delta u_1(\mathbf{r}_1)\,\delta u_1(\mathbf{r}_2)}=\rho_2^F(u_1\,|\,\mathbf{r}_1,\mathbf{r}_2)-\rho_1^F(u_1\,|\,\mathbf{r}_1)\rho_1^F(u_1\,|\,\mathbf{r}_2)\ . \tag{2.9}$$

Our notation should bring to mind the explicit dependence of the densities on the one-body attenuation factor $u_1(\mathbf{r})$. The superscript F indicates that the two-body correlations are switched off. For the calculation of the generating functional G_F by means of a cluster expansion,

$$G_F=\sum_n(\delta G_F)_n\ , \tag{2.10}$$

we have to assume that the system is localized and that the single-particle orbitals are asymptotically exact, i.e., that $u_1(\mathbf{r})\to 0$ as $r\to\infty$. Then we may expand in powers of the function $h_1(\mathbf{r})\equiv\exp[u_1(\mathbf{r})]-1$. The first terms in this expansion, from which we can see the general principle, are

$$(\delta G_F)_1=\sum_i\langle i\,|\,h_1(\mathbf{r})\,|\,i\rangle=\int d^3r\,h_1(\mathbf{r})\rho_1^F(\mathbf{r},\mathbf{r})\ , \tag{2.11}$$

$$\begin{aligned}(\delta G_F)_2&=\frac{1}{2!}\sum_{i,j}[\langle ij\,|\,h_1(\mathbf{r}_1)h_1(\mathbf{r}_2)\,|\,ij\rangle_a-\langle i\,|\,h_1(\mathbf{r})\,|\,i\rangle\langle j\,|\,h_1(\mathbf{r})\,|\,j\rangle]\\&=-\frac{1}{2}\sum_{i,j}\langle ij\,|\,h_1(\mathbf{r}_1)h_1(\mathbf{r}_2)\,|\,ji\rangle=-\frac{1}{2\nu}\int d^3r_1\,d^3r_2\,h_1(\mathbf{r}_1)h_1(\mathbf{r}_2)\rho_1^F(\mathbf{r}_1,\mathbf{r}_2)\rho_1^F(\mathbf{r}_2,\mathbf{r}_1)\ ,\end{aligned} \tag{2.12}$$

$$\begin{aligned}(\delta G_F)_3&=\frac{1}{3!}\sum_{i,j,k}[\langle ijk\,|\,h_1(\mathbf{r}_1)h_1(\mathbf{r}_2)h_1(\mathbf{r}_3)\,|\,ijk\rangle_a-3\langle ij\,|\,h_1(\mathbf{r}_1)h_1(\mathbf{r}_2)\,|\,ij\rangle_a\langle k\,|\,h_1(\mathbf{r})\,|\,k\rangle\\&\qquad+2\langle i\,|\,h_1(\mathbf{r})\,|\,i\rangle\langle j\,|\,h_1(\mathbf{r})\,|\,j\rangle\langle k\,|\,h_1(\mathbf{r})\,|\,k\rangle]\\&=\frac{1}{3}\sum_{i,j,k}\langle ijk\,|\,h_1(\mathbf{r}_1)h_1(\mathbf{r}_2)h_1(\mathbf{r}_3)\,|\,jki\rangle\\&=\frac{1}{3\nu^2}\int d^3r_1\,d^3r_2\,d^3r_3\,h_1(\mathbf{r}_1)h_1(\mathbf{r}_2)h_1(\mathbf{r}_3)\rho_1^F(\mathbf{r}_1,\mathbf{r}_2)\rho_1^F(\mathbf{r}_2,\mathbf{r}_3)\rho_1^F(\mathbf{r}_3,\mathbf{r}_1)\ .\end{aligned} \tag{2.13}$$

In Eqs. (2.11)–(2.13) we have abbreviated the single-particle orbitals $\phi_i(\mathbf{r})\mathcal{X}(i)$ by their labels i. ν is the degree of degeneracy of the single-particle states, and

$$\rho_1^F(\mathbf{r}_i,\mathbf{r}_j)\equiv\sum_k n(k)\phi_k^*(\mathbf{r}_i)\phi_k(\mathbf{r}_j) \tag{2.14}$$

is the one-body density matrix of the model system. The subscript a indicates antisymmetrization; $n(k)$ is the occupation number of the kth orbital. The sequence of approximants (2.11)–(2.13) to the generating functional G_F reveals the general formation law which may be verified, with increasing complexity, at higher orders of the cluster expansion (2.10):

$$G_F=\sum_{n=1}^{\infty}\frac{(-\nu)^{1-n}}{n}\int d^3r_1\cdots d^3r_n\,h_1(\mathbf{r}_1)\cdots h_1(\mathbf{r}_n)\times\rho_1^F(\mathbf{r}_1,\mathbf{r}_2)\cdots\rho_1^F(\mathbf{r}_n,\mathbf{r}_1)\ . \tag{2.15}$$

We are now ready to construct, via Eqs. (2.8) and (2.9), the one-, two-, . . . , n-body densities by functional variation. We introduce a shorthand notation for convolution products of two-point functions. For a pair of two-point functions $A(\mathbf{r}_1,\mathbf{r}_2)$ and $B(\mathbf{r}_1,\mathbf{r}_2)$ we define

$$[A*B](\mathbf{r}_1,\mathbf{r}_2)\equiv\int d^3r_3\,A(\mathbf{r}_1,\mathbf{r}_3)B(\mathbf{r}_3,\mathbf{r}_2)\ . \tag{2.16}$$

Functions of one variable are interpreted as diagonal, i.e., $h_1(\mathbf{r})\equiv h_1(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')$. We find

$$\rho_1^F(u_1\,|\,\mathbf{r})=[1+h_1(\mathbf{r})]\left[\rho_1^F(\mathbf{r},\mathbf{r})-\frac{1}{\nu}[\rho_1^F*h_1*\rho_1^F](\mathbf{r},\mathbf{r})+\frac{1}{\nu^2}[\rho_1^F*h_1*\rho_1^F*h_1*\rho_1^F](\mathbf{r},\mathbf{r})-\cdots\right]\equiv\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r})\ , \tag{2.17}$$

where we have defined a generalized one-body density matrix,

$$\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r}')\equiv\sqrt{1+h_1(\mathbf{r})}\left[\rho_1(\mathbf{r},\mathbf{r}')-\frac{1}{\nu}[\rho_1^F*h_1*\rho_1^F](\mathbf{r},\mathbf{r}')+\frac{1}{\nu^2}[\rho_1^F*h_1*\rho_1^F*h_1*\rho_1^F](\mathbf{r},\mathbf{r}')-\cdots\right]\sqrt{1+h_1(\mathbf{r}')}\ . \tag{2.18}$$

[Note that $\rho_1^F(u_1=0\,|\,\mathbf{r},\mathbf{r}')\equiv\rho_1^F(\mathbf{r},\mathbf{r}')$.]

The higher-order distribution functions are conveniently expressed in terms of the generalized one-body density matrix $\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r}')$. They assume a form which is structurally identical to the form of these functions in the absence of the one-body correlation factor. In particular we have

$$\rho_2^F(u_1\,|\,\mathbf{r},\mathbf{r}')=\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r})\rho_1^F(u_1\,|\,\mathbf{r}',\mathbf{r}') - \frac{1}{\nu}\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r}')\rho_1^F(u_1\,|\,\mathbf{r}',\mathbf{r}) \; . \tag{2.19}$$

It is important to note that the generalized density matrix $\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r}')$ preserves all properties of the noninteracting system which are important for the structure of the cluster expansions to be discussed in the next section. These properties are the following:

(i) The generalized density matrix preserves the particle number, i.e.,

$$\int d^3r\,\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r})=\int d^3r\,\rho_1^F(u_1=0\,|\,\mathbf{r},\mathbf{r}) \; . \tag{2.20}$$

(ii) The generalized density matrix is a projection operator in the sense of the above convolution product definition, i.e.,

$$[\rho_1^F(u_1)*\rho_1^F(u_1)](\mathbf{r},\mathbf{r}')=\nu\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r}') \; . \tag{2.21}$$

(iii) The generalized density matrix has a spectral representation,

$$\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r}')=\sum_i n(i)\psi_i^*(u_1\,|\,\mathbf{r})\psi_i(u_1\,|\,\mathbf{r}') \; , \tag{2.22}$$

where the $\psi_i(u_1\,|\,\mathbf{r})$ are a set of single-particle wave functions, i.e., $\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r}')$ is in fact for all $u_1(\mathbf{r})$ the density matrix of a model system described by the Slater determinant of single-particle orbitals $\psi_i(u_1\,|\,\mathbf{r})$.

Properties (i) and (ii) are easily proven by direct evaluation using that $\rho_1^F(u_1=0\,|\,\mathbf{r},\mathbf{r}')$ is a projection operator. Property (iii) is just the spectral representation of a projection operator.

III. CLUSTER EXPANSIONS FOR INHOMOGENEOUS FERMI SYSTEMS

The next task in the development of a variational theory for inhomogeneous systems is the derivation of cluster expansion and summation methods for the interesting physical quantities. We start again with the generating functional

$$G=\ln\left\langle\Phi_0\left|\exp\left[\sum_i u_1(\mathbf{r}_i)+\sum_{i<j}u_2(\mathbf{r}_i,\mathbf{r}_j)\right]\right|\Phi_0\right\rangle \; . \tag{3.1}$$

The derivation of the cluster expansion

$$G=\sum_n(\Delta G)_n \tag{3.2}$$

for variational wave functions (1.2) is presently a technical exercise; the usual diagrammatic notation[11] (see also Ref. 12) can be carried over to the inhomogeneous case with only slight modifications. Cluster contributions to the generating functional G and related quantities are represented as diagrams using the following graphical elements:

(i) Small open circles ("external" or "reference" points) represent the coordinates of particles. Filled circles ("internal" or "field" points) involve an integration over the coordinate space of that particle and a spin sum. We deviate here from the usual convention which includes a density factor.

(ii) Dashed lines ("correlation lines") between two circles i and j represent dynamical correlations $h_2(\mathbf{r}_i,\mathbf{r}_j)=\exp[u_2(\mathbf{r}_i,\mathbf{r}_j)]-1$.

(iii) Solid, oriented lines from point i to point j represent one-body density matrices ("exchange lines") $\rho_1^F(u_1\,|\,\mathbf{r}_i,\mathbf{r}_j)$.

The expansion of G in terms of correlation functions and exchange functions (one-body density matrices) is represented by the set of all topologically distinct connected diagrams without external points constructed after the following rules:

(iv) Each n-body diagram has a counting factor $1/n!$.

(v) Each point is attached by at least one correlation line $h_2(\mathbf{r}_i,\mathbf{r}_j)$. Two different points may be connected by at most one correlation factor.

(vi) Each point is attached by exactly one incoming and one outgoing exchange line.

(vii) Exchange lines occur always in closed polygons and carry a factor $(-\nu)^{1-n}$, where n is the number of points connected by the exchange loop.

The single-particle orbitals $\phi_i(\mathbf{r}_j)\chi(i)$ and the attenuation factor $u_1(\mathbf{r})$ appear in the diagrammatic expansion only in $\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r}')$. We have to keep the functional dependence of $\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r}')$ on $u_1(\mathbf{r})$ in mind when we calculate distribution functions by functional variation; i.e., we must observe [cf. Eqs. (2.8), (2.9), and (2.18)]

$$\frac{\delta\rho_1^F(u_1\,|\,\mathbf{r}_1,\mathbf{r}_2)}{\delta u_1(\mathbf{r})}=\tfrac{1}{2}\rho_1^F(u_1\,|\,\mathbf{r}_1,\mathbf{r}_2)[\delta(\mathbf{r}_1-\mathbf{r})+\delta(\mathbf{r}-\mathbf{r}_2)] - \frac{1}{\nu}\rho_1^F(u_1\,|\,\mathbf{r}_1,\mathbf{r})\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r}_2) \; . \tag{3.3}$$

We show in Fig. 1 all cluster contributions to G having one or two correlation factors $h_2(\mathbf{r}_i,\mathbf{r}_j)$. The essential new feature compared to the theory of the bulk system is that the expansion is reducible (diagrams 3, 5, 7, and 8 of Fig. 1). Otherwise, the same topological rules apply. In the limit of the bulk system, the reducible diagrams cancel due to momentum conservation.

The second step in the development of a variational theory is the calculation of distribution functions and the classification of (topologically defined) subsets of diagrams which may be summed by integral-equation methods. These subsets serve then for a compact representation of physical quantities of interest. To find such classifications we study first the one-body density $\rho_1(\mathbf{r})$ which is obtained by functional variation

$$\rho_1(\mathbf{r})=\frac{\delta G}{\delta u_1(\mathbf{r})} \; , \tag{3.4}$$

observing (3.3). The graphical representation of the first few diagrams contributing to $\rho_1(\mathbf{r})$ is shown in Fig. 2. Note that the volume integral of all correction terms to the "Hartree-Fock" density $\rho_1^F(\mathbf{r},\mathbf{r})$ (first diagram in Fig.

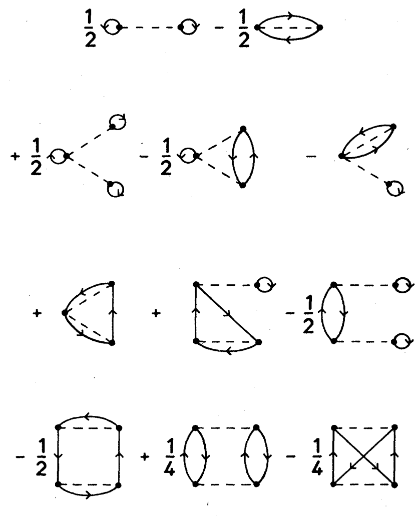

FIG. 1. All diagrams in the diagrammatic representation of the cluster expansion (3.2) are shown which contain one or two correlation lines. Diagrams 3, 5, 7, and 8 are reducible.

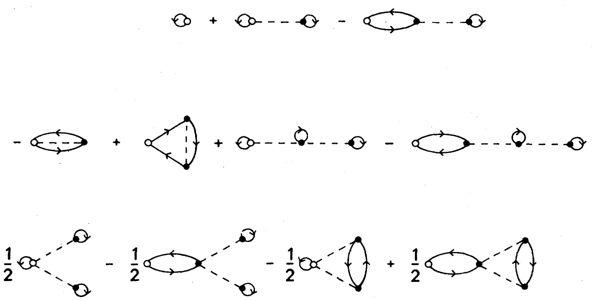

FIG. 2. Graphical representation of the first few terms in the cluster-expansion of the one-body density. The first diagram is the Hartree-Fock density, diagrams 2, 3, and 6—11 are included in the definition of the generalized density matrix $\rho_1^F(u_\gamma\,|\,\mathbf{r}_i,\mathbf{r}_j)$, cf. Eq. (3.5). Note that the exchange line contains the one-body attenuation factor $u_1(\mathbf{r})$, i.e., it represents the function $\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r}')$, cf. Eq. (2.18).

2) vanishes due to the convolution property (2.21).

One class of contributions to $\rho_1(\mathbf{r})$ includes those which can be written in the form $\rho_1^F(u_1\,|\,\mathbf{r},\mathbf{r})\{\exp[\gamma(\mathbf{r})]-1\}$. Diagrams 2, 6, 8, and 10 of Fig. 2 belong to this class. The same subset of diagrams which generates the factor $\{\exp[\gamma(\mathbf{r})]-1\}$ may be connected through an exchange loop to the reference point; examples of such structures are diagrams 3, 7, 9, and 11 of Fig. 2. In fact, we may connect any number of such sets of diagrams by a single exchange path with the reference point $\mathbf{r}$. A more complicated example is shown in Fig. 3. The same construction may be applied at any internal point and results in a second "dressing" of the exchange factor of the same form as discussed in Eq. (2.18), but with $u_1(\mathbf{r})$ replaced by $\gamma(\mathbf{r})$. Graphically, $\{\exp[\gamma(\mathbf{r})]-1\}$ is the set of all diagrams with one reference point $\mathbf{r}$, having no exchange line attached to that point. Blending the two consecutive dressings, we are led to the final form of the "dressed" one-body density matrix

$$\rho_1^F(u_1+\gamma\,|\,\mathbf{r},\mathbf{r}')=\sqrt{1+h_\gamma(\mathbf{r})}\left[\rho_1^F(u_1=0\,|\,\mathbf{r},\mathbf{r}')-\frac{1}{\nu}[\rho_1^F(u_1=0)*h_\gamma*\rho_1^F(u_1=0)](\mathbf{r},\mathbf{r}')-\cdots\right]\sqrt{1+h_\gamma(\mathbf{r}')}\;, \tag{3.5}$$

where we have abbreviated

$$h_\gamma(\mathbf{r})\equiv\exp[u_1(\mathbf{r})+\gamma(\mathbf{r})]-1\equiv\exp[u_\gamma(\mathbf{r})]-1\;. \tag{3.6}$$

From now on we will use the oriented solid line to represent the fully dressed density matrix $\rho_1^F(u_\gamma\,|\,\mathbf{r},\mathbf{r}')$, and omit in our graphical representation the sets of diagrams summed in this function.

In terms of the dressed exchange factor $\rho_1^F(u_\gamma\,|\,\mathbf{r},\mathbf{r}')$, the graphical expansion of the physical one-body density becomes rather compact. The leading term, which integrates to the total particle number, is simply the generalized Hartree-Fock density $\rho_1^F(u_\gamma\,|\,\mathbf{r},\mathbf{r})$. The only remaining first-order terms are diagrams 4 and 5 of Fig. 2. These two diagrams, and proper combinations of higher-order diagrams, integrate pairwise to zero. The rules for the representation of the generating functional G are a bit more complicated; see Ref. 9 for details.

IV. ENERGY EXPECTATION VALUE AND OPTIMAL ONE-BODY CORRELATIONS

The energy expectation value is the key to the variational determination of the one- and two-body correlations. We assume a many-body system of particles in an external field $U_{\mathrm{ext}}(\mathbf{r})$, interacting via a local two-body potential $v(r)$, i.e., the Hamiltonian is

$$H=-\frac{\hbar^2}{2m}\sum_i\nabla_i^2+\sum_i U_{\mathrm{ext}}(\mathbf{r}_i)+\sum_{i<j}v(\,|\,\mathbf{r}_i-\mathbf{r}_j\,|\,)\;. \tag{4.1}$$

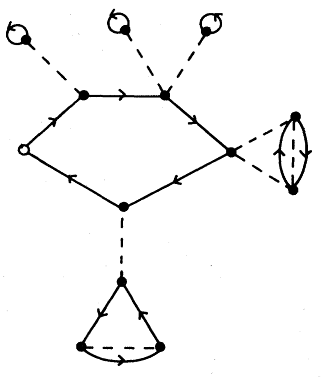

FIG. 3. A more complicated example of reducible diagrams contained in the generalized density matrix $\rho_1(u_\gamma\,|\,\mathbf{r},\mathbf{r})$.

To a large extent we can rely on results of optimization procedures of homogeneous quantum liquids, which may be summarized in the two following statements:

(1) The hypernetted-chain approximation is the simplest approximation for the distribution functions and the energy expectation value which preserves the qualitative structure of the exact Euler-Lagrange equation.[6]

(2) The Jackson-Feenberg treatment of the kinetic energy[3] is necessary to guarantee the existence of local minima.[13]

It is not yet necessary to make explicit use of a specific method like the FHNC to relate the two-body density to the pair correlation factor. Rather, we concentrate here on the optimal determination of the single-particle basis. Using the Jackson-Feenberg identity

$$F\nabla^2 F=\tfrac{1}{2}(F^2\nabla^2+\nabla^2F^2)+\tfrac{1}{2}F^2[\nabla,[\nabla,\ln F]] -\tfrac{1}{4}[\nabla,[\nabla,F^2]] \tag{4.2}$$

we find with $T\equiv-(\hbar^2/2m)\sum_i\nabla_i^2$,

$$E=T_F+E_1^*+E_2^*+T_{\mathrm{JF}}^* , \tag{4.3}$$

where

$$T_F=\frac{1}{2}\frac{\langle\Phi_0|(TF^2+F^2T)|\Phi_0\rangle}{\langle\Phi_0|F^2|\Phi_0\rangle}=-\frac{\hbar^2}{4m}\int d^3r(\nabla^2_{F\,\mathrm{in}}+\nabla^2_{F\,\mathrm{out}})\rho_1(\mathbf{r}) , \tag{4.4}$$

$$E_1^*=\left\langle\Psi_0\left|\sum_i\left[U_{\mathrm{ext}}(\mathbf{r}_i)-\frac{\hbar^2}{8m}\nabla^2u_1(\mathbf{r}_i)\right]\right|\Psi_0\right\rangle=\int d^3r\,\rho_1(\mathbf{r})\left[U_{\mathrm{ext}}(\mathbf{r})-\frac{\hbar^2}{8m}\nabla^2u_1(\mathbf{r})\right] , \tag{4.5}$$

$$\begin{aligned}E_2^*&=\left\langle\Psi_0\left|\sum_{i<j}\left[v(|\mathbf{r}_i-\mathbf{r}_j|)-\frac{\hbar^2}{8m}(\nabla_i^2+\nabla_j^2)u_2(\mathbf{r}_i,\mathbf{r}_j)\right]\right|\Psi_0\right\rangle\\&=\tfrac{1}{2}\int d^3r_1\,d^3r_2\,\rho_2(\mathbf{r}_1,\mathbf{r}_2)\left[v(|\mathbf{r}_1-\mathbf{r}_2|)-\frac{\hbar^2}{8m}(\nabla_1^2+\nabla_2^2)u_2(\mathbf{r}_1,\mathbf{r}_2)\right] ,\end{aligned} \tag{4.6}$$

and

$$T_{\mathrm{JF}}^*=\frac{\hbar^2}{8m}\left\langle\Psi_0\left|\sum_i\frac{\nabla_i^2F^2}{F^2}\right|\Psi_0\right\rangle=\frac{\hbar^2}{8m}\int d^3r\,\nabla_F^2\rho_1(\mathbf{r}) . \tag{4.7}$$

The last expressions in Eqs. (4.4) and (4.7) are written in a somewhat symbolic form and are to be interpreted graphically: In a diagrammatic representation of the function it acts on, the operator $\nabla_{F\,\mathrm{in}}$ differentiates only the *incoming* exchange factor $\rho_F(\mathbf{r},\mathbf{r}')$ in point $\mathbf{r}$, whereas the operator $\nabla_{F\,\mathrm{out}}$ differentiates the *outgoing* exchange function, and

$$\nabla_F=\nabla_{F\,\mathrm{in}}+\nabla_{F\,\mathrm{out}} . \tag{4.8}$$

In the Bose case, the function $u_1(\mathbf{r})$ would be eliminated in favor of the physical one-body density $\rho_1(\mathbf{r})$ by the Born-Green-Yvon (BGY) equation. A similar transformation of the independent one-body function must be made in the case of Fermi statistics. The Fermi generalization of the BGY equation is

$$\nabla\rho_1(\mathbf{r})=\rho_1(\mathbf{r})\nabla u_1(\mathbf{r})+\int d^3r'\rho_2(\mathbf{r},\mathbf{r}')\nabla_r u_2(\mathbf{r},\mathbf{r}')+\nabla_F\rho_1(\mathbf{r}) . \tag{4.9}$$

The term $\nabla_F\rho_1(\mathbf{r})$ should again be understood in the diagrammatic sense outlined above. Equation (4.9) may be derived in a manner similar to the derivation of the two-body BGY equations for Fermi systems.[14] Using (4.9), we can write the energy expectation value in the form

$$E=T_F+E_1+E_2+T_{\mathrm{JF}} , \tag{4.10}$$

with

$$\begin{aligned}E_1&=\int d^3r\,\rho_1(\mathbf{r})U_{\mathrm{ext}}(\mathbf{r}) ,\\E_2&=\tfrac{1}{2}\int d^3r\,d^3r'\,\rho_2(\mathbf{r},\mathbf{r}')v_{\mathrm{JF}}(\mathbf{r},\mathbf{r}') ;\end{aligned} \tag{4.11}$$

$$v_{\mathrm{JF}}(\mathbf{r},\mathbf{r}')=v(|\mathbf{r}-\mathbf{r}'|)-\frac{\hbar^2}{8m}[\rho_1^{-1}(\mathbf{r})\nabla_r\rho_1(\mathbf{r})\cdot\nabla_r+\rho_1^{-1}(\mathbf{r}')\nabla_{r'}\rho_1(\mathbf{r}')\cdot\nabla_{r'}]u_2(\mathbf{r},\mathbf{r}') , \tag{4.12}$$

$$T_{\mathrm{JF}}=\frac{\hbar^2}{8m}\int d^3r\{\nabla\ln\rho_1(\mathbf{r})\cdot[\nabla\rho_1(\mathbf{r})-\nabla_F\rho_1(\mathbf{r})]+\nabla_F^2\rho_1(\mathbf{r})\} . \tag{4.13}$$

Finally, we can single out the proper one-body pieces of $T_F+E_1+T_{\mathrm{JF}}$, i.e., all those terms in which the full one-body density is replaced by the generalized Hartree density $\rho_1^F(u_\gamma\,|\,\mathbf{r},\mathbf{r})$:

$$T_F+E_1+T_{\mathrm{JF}}\equiv(\Delta E)^{(1)}+(\Delta E_1)^{(2)}+(\Delta T_{\mathrm{JF}})^{(2)}\equiv(\Delta E)^{(1)}+(\Delta E)^{(2)}\ , \tag{4.14}$$

with

$$(\Delta E)^{(1)}=\int d^3r\left[\rho_1^F(u_\gamma\,|\,\mathbf{r},\mathbf{r})U_{\mathrm{ext}}(\mathbf{r})+\frac{\hbar^2}{8m}\nabla\rho_1^F(u_\gamma\,|\,\mathbf{r},\mathbf{r})\cdot\nabla u_\gamma(\mathbf{r})-\frac{\hbar^2}{4m}(\nabla^2_{F\,\mathrm{in}}+\nabla^2_{F\,\mathrm{out}}-\tfrac{1}{2}\nabla^2_F)\rho_1^F(u_\gamma\,|\,\mathbf{r},\mathbf{r})\right]\ . \tag{4.15}$$

[We have combined higher-order contributions to T_F and E_1 in $(\Delta E_1)^{(2)}$.]

The next task is the choice of the one-body variable which we consider as the independent variational coordinate. In the Bose case, the one-body density has been chosen as the independent one-body function. One cannot go quite so far in the Fermi case, since $\rho_1(\mathbf{r})$ is still expressed in terms of a sum of diagrams. The most natural choice of the independent one-body function is the set of diagrams summed in $u_\gamma(\mathbf{r})$, and we will see that the choice of this quantity as the independent one-body function is the most practical one.

Let us recall the proof of Secs. II and III that the one-body quantity $u_\gamma(\mathbf{r})$ may always be eliminated by a suitable transformation of the single-particle basis. Hence, the optimal $u_\gamma(\mathbf{r})$ depends solely on the choice of the single-particle basis. We may therefore think of a procedure which determines first, from an original set of single-particle functions $\phi_i(\mathbf{r})$, the optimal $u_\gamma(\mathbf{r})$ by minimization of the ground-state energy. Thereafter, a basis transformation is performed which eliminates the optimal $u_\gamma(\mathbf{r})$. Another way to phrase the same procedure is: *Find the set of single-particle orbitals such that the optimal one-body factor* $u_\gamma(\mathbf{r})$ *vanishes, i.e., such that the equation*

$$\frac{\delta E}{\delta u_\gamma(\mathbf{r})}=0 \tag{4.16}$$

has the solution

$$u_\gamma^{\mathrm{opt}}(\mathbf{r})=0\ . \tag{4.17}$$

The optimization of one one-body function gives a necessary condition for the basis but does not uniquely determine the single-particle states. The remaining flexibility allows the single-particle states to be determined from a generalized Hartree-Fock one-body Hamiltonian.

The calculation of the variational derivative (4.16) at $u_\gamma(\mathbf{r})=0$ leads to a number of substantial simplifications. Carrying out the variation (4.16) and inserting the definition (2.14) for the Slater function $\rho_1^F(u_\gamma=0\,|\,\mathbf{r},\mathbf{r}')$ leads to the constraint

$$\sum_i n(i)\int d^3r_1\left[\left[-\frac{\hbar^2}{2m}\nabla^2+U_{\mathrm{ext}}(\mathbf{r}_1)\right]\phi_i(\mathbf{r}_1)+\int d^3r_2\frac{\delta((\Delta E)^{(2)}+E_2)}{\delta\rho_1^F(u_1=0\,|\,\mathbf{r}_1,\mathbf{r}_2)}\phi_i(\mathbf{r}_2)\right]\left[\delta(\mathbf{r}-\mathbf{r}_1)-\frac{1}{\nu}\rho_F(\mathbf{r},\mathbf{r}_1)\right]+\mathrm{c.c.}=0\ . \tag{4.18}$$

Equation (4.18) is solved by a set of single-particle states determined by

$$\left[-\frac{\hbar^2}{2m}\nabla^2+U_{\mathrm{ext}}(\mathbf{r})\right]\phi_i(\mathbf{r})+\int d^3r_1\frac{\delta((\Delta E)^{(2)}+E_2)}{\delta\rho_1^F(u_1=0\,|\,\mathbf{r},\mathbf{r}_1)}\phi_i(\mathbf{r}_1)=\epsilon_i\phi_i(\mathbf{r})\ , \tag{4.19}$$

which is the generalized Hartree-Fock equation within the variational theory. Note that Eq. (4.19) reduces to the ordinary Hartree-Fock equation in the limit that the two-body correlation factor $u_2(\mathbf{r},\mathbf{r}')$ vanishes. Equation (4.19) is quite plausible, and the determination of the single-particle orbitals through Eq. (4.19) leads automatically to the most compact form of the cluster expansions and the FHNC equations. We may now invoke the usual arguments of Hartree-Fock theory to show that the generalized Hartree-Fock basis generated by Eq. (4.19) minimizes the energy expectation value in the space of *all* correlated wave functions where the model state $|\Phi_0\rangle$ is a single Slater determinant.

We should draw here briefly the connection to a related approach by Ripka,[9] who suggested the elimination of the reducible diagrams by an *ad hoc* choice of the one-body attenuation factor $u_1(\mathbf{r})$. Our work clarifies and extends this approach in a number of aspects.

(i) Given an *ad hoc* choice of the single-particle basis, one is usually not at liberty to choose an arbitrary one-body attenuation factor $u_1(\mathbf{r})$ without violating the cluster property of the optimal $u_2(\mathbf{r},\mathbf{r}')$.

(ii) The renormalized attenuation factor $u_\gamma(\mathbf{r})$ may always be eliminated by a suitable basis transformation.

(iii) An explicit scheme for the derivation of that single-particle basis has been given.

V. FERMI-HYPERNETTED-CHAIN EQUATIONS FOR INHOMOGENEOUS SYSTEMS

The optimal determination of the single-particle orbitals discussed in the preceding section results in significant simplifications of the cluster expansion (3.2) for the generating functional and the one- and two-body distribution functions. We will now take advantage of these simplifications and omit all diagrams which can be chosen to vanish by the optimal single-particle basis generated by the generalized Hartree-Fock equation (4.19). From now on we identify

$$\rho_1^F(u_\gamma^{\mathrm{opt}}=0\,|\,\mathbf{r},\mathbf{r}')\equiv\rho_1^F(\mathbf{r},\mathbf{r}')\ . \tag{5.1}$$

For the calculation of distribution functions through the algorithms (3.4) and

$$\rho_2(\mathbf{r},\mathbf{r}')=\frac{\delta^2 G}{\delta u_1(\mathbf{r})\,\delta u_1(\mathbf{r}')}+\rho_1(\mathbf{r})\rho_1(\mathbf{r}') , \tag{5.2}$$

one must still observe (3.3). Our next task in the development of the variational theory of inhomogeneous Fermi systems is the derivation of integral equations summing, for a given two-body correlation factor $u_2(\mathbf{r},\mathbf{r}')$, infinite series of cluster contributions to the two-body density. Experience in the theory of homogeneous Fermi fluids[6] and inhomogeneous Bose systems[1] establishes the Fermi-hypernetted-chain (FHNC) approximation[5] as the minimum requirement.

Attempts to generalize the FHNC theory to inhomogeneous systems were some time ago reported by Fantoni[15] and by Ripka.[9] Both treatments are not immediately applicable: It has been known for some time[5] that even the bulk limit of the "FHNC" equations derived in Ref. 15 is problematic in the sense that it violates the Pauli principle in the intermediate states. The ailments of that theory are enhanced in the more complicated inhomogeneous case. We will derive below consistency conditions which must be met in expansions of the one-body density in order to conserve the particle number, and between one-body and two-body densities in order to guarantee the correct normalization, sequential relations, and long-wavelength properties. These consistency requirements were the guiding principle in the derivation of the FHNC equations of Ref. 5.

Care is needed to construct consistent approximation schemes for the one-body and the two-body functions. Consider the sequential relation between the one-body and the two-body density,

$$-\rho_1(\mathbf{r}_1)=\int d^3r_2[\rho_2(\mathbf{r}_1,\mathbf{r}_2)-\rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2)] . \tag{5.3}$$

We show in Fig. 4 all diagrams contributing to $\rho_2(\mathbf{r}_1,\mathbf{r}_2)-\rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2)$ containing no or one correlation factor. Performing the integral (5.3) we see that the first diagram shown in Fig. 4 (i.e., the one containing no correlation factor) integrates to the generalized Hartree-Fock density $\rho_1^F(\mathbf{r},\mathbf{r})$. The remaining diagrams integrate to the contributions to $\rho_1(\mathbf{r})$ containing one correlation factor, i.e., to the diagrams 4 and 5 in Fig. 2.

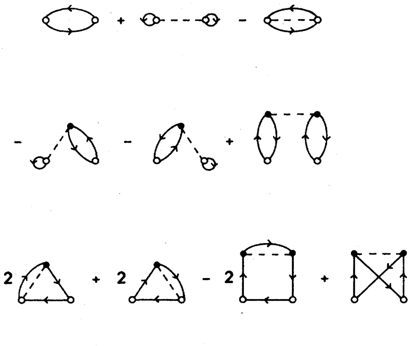

FIG. 4. Diagrammatic representation of all diagrams contributing to the two-body density $\rho_2(\mathbf{r}_1,\mathbf{r}_2)$ containing no more than one correlation line. Note that we assume that the one-body density matrix (solid, oriented line) is the one obtained from the optimized single-particle basis.

We see that consistent approximations must be made for the one- and two-body densities in order to guarantee the sequential relation (5.3). A possible, but not unique, guiding principle is to classify the cluster contributions according to the number of correlation lines involved. We note also that the present consideration is just one consistency requirement. In a strongly interacting system one will also require that the two-body density is proportional to $1+h_2(\mathbf{r},\mathbf{r}')$. Both of the above requirements can be satisfied rigorously only by the summation of an infinite series of three- and four-point diagrams,[6] one has to either resort to approximations or accept a slight inconsistency between the two-body density and the static form factor.

The request for consistent approximation schemes for the one- and two-body quantities is a more general one to be observed in the derivation of integral equation techniques. Consider the chaining operation of two dynamical bonds $h_2(\mathbf{r}_i,\mathbf{r}_j)$, see Fig. 5. Diagrams 1 and 4 shown in Fig. 5 represent the two simplest ways of "chaining." The topological structure is reminiscent of the RPA ring diagrams, as may be seen easily by realizing that these two diagrams can be combined in the form

$$\int d^3r_1\, d^3r_2\, h_2(\mathbf{r},\mathbf{r}_1) \times \sum_{ij} n(i)[1-n(j)]\psi_i(\mathbf{r}_1)\psi_i^*(\mathbf{r}_2)\psi_j(\mathbf{r}_2)\psi_j^*(\mathbf{r}_1)h_2(\mathbf{r}_2,\mathbf{r}') . \tag{5.4}$$

In other words, the decomposition of the combination (5.4) into two different diagrams is simply the decomposition of the projection operator $1-n(j)$ on the particle states into a unit operator *minus* a projection operator on the hole states. Of course, the two diagrams must be kept together.

The remaining diagrams shown in Fig. 5 depict all corrections to the chaining operation which contain one two-body correlation factor. Diagrams 2 and 3 show the first-order corrections to the generalized Hartree-Fock density $\rho_1^F(\mathbf{r},\mathbf{r})$ (cf. Fig. 2). The other ones may be identified with "propagator corrections." A representation similar to (5.4) in terms of projection operators may be introduced.[16] Using the convolution property (2.21), it is readily shown that the volume integral of the two-point function connecting the dynamical bonds $h_2(\mathbf{r}_i,\mathbf{r}_j)$ in diagrams 5—9 of Fig. 5, equals the first-order correction term to the one-body density with opposite sign. Hence,

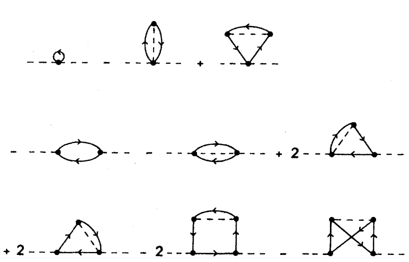

FIG. 5. Simplest insertions to the chaining of two dynamical bonds.

in a systematic approximation scheme which preserves the long-wavelength properties of the expansion, the first-order corrections should either all be kept, or all be neglected. This is the generalization of the FHNC scheme derived in Ref. 5.

With these preliminary remarks, we are ready to formulate the norm-conserving FHNC equations for an inhomogeneous system. We will formulate these equations at the simplest level which is sufficient for a satisfactory implementation of an optimization procedure. To be specific, we neglect all propagator corrections (i.e., the diagrams 5—9 in Fig. 5 and their generalizations). For consistency, the density is then the optimized Hartree-Fock density $\rho_1^F(\mathbf{r},\mathbf{r})$. In this approximation, the link between two dynamical correlation bonds is simply the Hartree-Fock static form factor,

$$S_F(\mathbf{r}_1,\mathbf{r}_2)=\delta(\mathbf{r}_1-\mathbf{r}_2)-\frac{1}{\nu}\frac{|\rho_1^F(\mathbf{r}_1,\mathbf{r}_2)|^2}{[\rho_1^F(\mathbf{r}_1,\mathbf{r}_1)\rho_1^F(\mathbf{r}_2,\mathbf{r}_2)]^{1/2}} . \tag{5.5}$$

The simplest consistent level of the FHNC equations may then be derived from the equations of Ref. 15 by systematic omission of all components which violate the Pauli principle unless "elementary" diagrams are included. We obtain a set of two equations for the "nodal" and "nonnodal" *dd* diagrams,

$$X_{dd}(\mathbf{r}_1,\mathbf{r}_2)\equiv\exp[u_2(\mathbf{r}_1,\mathbf{r}_2)+N_{dd}(\mathbf{r}_1,\mathbf{r}_2)]-1-N_{dd}(\mathbf{r}_1,\mathbf{r}_2) , \tag{5.6}$$

$$\hat{N}_{dd}(\mathbf{r}_1,\mathbf{r}_2)=[\hat{X}_{dd}*S_F*\hat{\Gamma}_{dd}](\mathbf{r}_1,\mathbf{r}_2) . \tag{5.7}$$

Here we have introduced for any two-point function $A(\mathbf{r}_1,\mathbf{r}_2)$ the abbreviation

$$\hat{A}(\mathbf{r}_1,\mathbf{r}_2)\equiv[\rho_1^F(\mathbf{r}_1,\mathbf{r}_1)]^{1/2}A(\mathbf{r}_1,\mathbf{r}_2)[\rho_1^F(\mathbf{r}_2,\mathbf{r}_2)]^{1/2} , \tag{5.8}$$

and

$$\Gamma_{dd}(\mathbf{r}_1,\mathbf{r}_2)\equiv X_{dd}(\mathbf{r}_1,\mathbf{r}_2)+N_{dd}(\mathbf{r}_1,\mathbf{r}_2) . \tag{5.9}$$

In the same approximation, the static form factor of the interacting system is

$$S(\mathbf{r}_1,\mathbf{r}_2)=S_F(\mathbf{r}_1,\mathbf{r}_2)+[S_F*\hat{\Gamma}_{dd}*S_F](\mathbf{r}_1,\mathbf{r}_2) . \tag{5.10}$$

The construction of a satisfactory pair correlation function requires some more thought in systems with a strongly repulsive core.[16–18] The representation (5.10) is sufficient for the electron gas in a metal surface.

VI. OPTIMAL PAIR CORRELATIONS

Using the optimal single-particle orbitals discussed in Sec. IV, the one-body part of the ground-state energy is simply the expectation value of the kinetic energy and the external potential in the Hartree-Fock basis,

$$(\Delta E)^{(1)}=\int d^3r\sum_i n(i)\phi_i^*(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2+U_{\text{ext}}(\mathbf{r})\right]\phi_i(\mathbf{r}) . \tag{6.1}$$

Note that there is no contribution from T_{JF} to $(\Delta E)^{(1)}$ in the optimized single-particle basis. The higher-order terms $(\Delta E_1)^{(2)}$ are conveniently expressed in the form

$$(\Delta E_1)^{(2)}=-\frac{1}{2\nu}\int d^3r\,d^3r_2\,\Gamma_{cc}(\mathbf{r}_1,\mathbf{r}_2)\left[(1-\rho_1^F/\nu)*\left[-\frac{\hbar^2}{2m}\nabla^2+U_{\text{ext}}\right]*\rho_1^F\right](\mathbf{r}_2,\mathbf{r}_1)+\text{c.c.} , \tag{6.2}$$

where $\Gamma_{cc}(\mathbf{r}_1,\mathbf{r}_2)$ is represented graphically by the set of all two-point diagrams having an exchange path going from the external point $\mathbf{r}_1$ to the external point $\mathbf{r}_2$. Its leading term is the Hartree-Fock density matrix $\rho_1^F(\mathbf{r}_1,\mathbf{r}_2)$; the contribution from this term integrates to zero. The next terms in a graphical expansion of $(\Delta E_1)^{(2)}$ are structurally similar to the corrections to the Hartree density and must be kept together with contributions to E_2 which include this density-correction term. Since we do not consider these terms in the present simplest version of the inhomogeneous FHNC-EL (Euler-Lagrange) theory, we have to ignore $(\Delta E_1)^{(2)}$ as well.

Similar simplifications arise for the kinetic energy T_{JF}: all one-body contributions vanish. Moreover, only contributions to T_{JF} survive in which the reference point $\mathbf{r}$ of the combinations $[\nabla\rho_1(\mathbf{r})-\nabla_F\rho_1(\mathbf{r})]$ and $\nabla_F^2\rho_1(\mathbf{r})$ is attached by at least one dynamical bond $h_2(\mathbf{r},\mathbf{r}')$. Recalling the topological structure of the expansion for the one-body density, we can represent T_{JF} in the form

$$T_{\text{JF}}=T_{\text{JF}}^{(2)}+T_{\text{JF}}^{(3)} , \tag{6.3}$$

$$T_{\text{JF}}^{(2)}=-\frac{\hbar^2}{8m\nu}\int d^3r_1d^3r_2\Gamma_{dd}(\mathbf{r}_1,\mathbf{r}_2)\nabla_1\left[\rho_1(\mathbf{r}_1)\cdot\nabla_1\frac{|\rho_1^F(\mathbf{r}_1,\mathbf{r}_2)|^2}{\rho_1(\mathbf{r}_1)}\right] , \tag{6.4}$$

and

$$T_{\text{JF}}^{(3)}=\frac{\hbar^2}{8m\nu^2}\int d^3r_1d^3r_2d^3r_3\Gamma_{dcc}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)\nabla_1\left[\rho_1(\mathbf{r}_1)\cdot\nabla_1\frac{\rho_1^F(\mathbf{r}_2,\mathbf{r}_1)\rho_1^F(\mathbf{r}_1,\mathbf{r}_3)}{\rho_1(\mathbf{r}_1)}\right] , \tag{6.5}$$

where[14] $\Gamma_{dcc}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$ is the set of all three-point diagrams having at least one dynamical bond $h_2(\mathbf{r}_1,\mathbf{r}_i)$ attached to point $\mathbf{r}_1$, and an exchange path going from point $\mathbf{r}_3$ to $\mathbf{r}_2$. The representations (6.3)—(6.5) of T_{JF} are suitable for the derivation of the Euler-Lagrange equations for the two-body correlations.

Just as is the case in the theory of bulk Fermi systems, it is convenient to consider separately the direct dependence of the energy on $u_2(\mathbf{r},\mathbf{r}')$ through the Jackson-Feenberg interaction, and independently its dependence through the distribution functions. The evaluation of both terms in the Euler equation $\delta E/\delta u_2(\mathbf{r}_1,\mathbf{r}_2)=0$ yields

$$\frac{\hbar^2}{8m}[\nabla_{r_1}\rho_1(\mathbf{r}_1)\cdot\nabla_{r_1}\rho_1^{-1}(\mathbf{r}_1)+\nabla_{r_2}\rho_1(\mathbf{r}_2)\cdot\nabla_{r_2}\rho_1^{-1}(\mathbf{r}_2)]\rho_2(\mathbf{r}_1,\mathbf{r}_2)=\int d^3r_3d^3r_4v_{\mathrm{JF}}(\mathbf{r}_3,\mathbf{r}_4)\frac{\delta\rho_2(\mathbf{r}_3,\mathbf{r}_4)}{\delta u_2(\mathbf{r}_1,\mathbf{r}_2)}+\frac{\delta T_{\mathrm{JF}}}{\delta u_2(\mathbf{r}_1,\mathbf{r}_2)}\equiv\rho_2'(\mathbf{r}_1,\mathbf{r}_2)\ . \tag{6.6}$$

The advantage of the representation (6.6) is that each term has its unique graphical definition, which allows an easy derivation of integral equations consistent with the level of FHNC approximation in which one chooses to work. For example, the first term in $\rho_2'(\mathbf{r}_1,\mathbf{r}_2)$ is generated graphically from the two-body density $\rho_2(\mathbf{r}_1,\mathbf{r}_2)$ by replacing, in turn, each correlation bond $h_2(\mathbf{r}_i,\mathbf{r}_j)$ by a screened Jackson-Feenberg interaction

$$[1+h_2(\mathbf{r}_i,\mathbf{r}_j)]v_{\mathrm{JF}}(\mathbf{r}_i,\mathbf{r}_j)\ .$$

The term $\delta T_{\mathrm{JF}}/\delta u_2(\mathbf{r}_1,\mathbf{r}_2)$ is generated by replacing, in turn, each connected pair of exchange functions $\rho_1^F(\mathbf{r}_j,\mathbf{r}_i)\rho_1^F(\mathbf{r}_i,\mathbf{r}_k)$ contributing to $\rho_2(\mathbf{r}_1,\mathbf{r}_2)$ by the combination

$$\frac{\hbar^2}{8m}\nabla_{r_i}\left[\rho_1(\mathbf{r}_i)\cdot\nabla_{r_i}\frac{\rho_1^F(\mathbf{r}_j,\mathbf{r}_i)\rho_1^F(\mathbf{r}_i,\mathbf{r}_k)}{\rho_1(\mathbf{r}_i)}\right]\ . \tag{6.7}$$

The determination of the optimal pair correlations in bulk Fermi systems is well understood and usually more efficient than the search for parametrized correlation functions. The most complete description of the optimization algorithm and the relevant equations may be found in Ref. 16; earlier applications[17,18] deviate from that by technical details. But the solution of the full FHNC—Euler-Lagrange (EL) problem involves the solution of eight coupled equations instead of two in the Bose case. In addition, inclusion or at least adequate estimates of Pauli-blocking effects are required to all orders. Considering the success of our Bose optimization,[1] such a calculation may well be desirable. We will refrain here from deriving the inhomogeneous FHNC-EL equations in all detail since the theory should be applied first at the simplest level that fulfills the consistency requirements set forth above. This is the simplest implementation of the FHNC scheme of Ref. 5; in other words, the FHNC approximation [(5.6)—(5.8)] in the inhomogeneous case. For consistency with the FHNC approximation [(5.6)—(5.8)], we must also assume $\rho_1(\mathbf{r})\equiv\rho_1^F(\mathbf{r},\mathbf{r})$.

In this approximation, the Jackson-Feenberg energy consists of just the first term $T_{\mathrm{JF}}^{(2)}$ given in Eq. (6.4).

We now formulate the FHNC′ equations for the generalized two-body density $\rho_2'(\mathbf{r}_1,\mathbf{r}_2)$. These equations correspond to the FHNC′ equations of Ref. 16; the simplifications introduced above have the effect that all "*de* diagrams" are neglected, and the "*ee* diagrams" are represented by the leading term in their expansion, which does not contain any correlation factors:

$$\begin{aligned}\rho_2'(\mathbf{r}_1,\mathbf{r}_2)=[\rho_1(\mathbf{r}_1)]^{1/2}[\rho_1(\mathbf{r}_2)]^{1/2}\{&[S*\hat{X}'_{dd}*S](\mathbf{r}_1,\mathbf{r}_2)\\&-\tfrac{1}{4}[(1+S_F*\hat{\Gamma}_{dd})*[H(1)*(S_F-1)+(S_F-1)*H(1)]*(1+\hat{\Gamma}_{dd}*S_F)](\mathbf{r}_1,\mathbf{r}_2)\}\ ,\end{aligned} \tag{6.8}$$

$$X'_{dd}(\mathbf{r}_1,\mathbf{r}_2)=[1+\Gamma_{dd}(\mathbf{r}_1,\mathbf{r}_2)]v_{\mathrm{JF}}(\mathbf{r}_1,\mathbf{r}_2)+\Gamma_{dd}(\mathbf{r}_1,\mathbf{r}_2)N'_{dd}(\mathbf{r}_1,\mathbf{r}_2)\ , \tag{6.9}$$

$$\begin{aligned}\hat{N}'_{dd}(\mathbf{r}_1,\mathbf{r}_2)=&[(1+\hat{\Gamma}_{dd}*S_F)*\hat{X}'_{dd}*(1+S_F*\hat{\Gamma}_{dd})-\hat{X}'_{dd}](\mathbf{r}_1,\mathbf{r}_2)\\&-\tfrac{1}{4}\{\hat{\Gamma}_{dd}*[H(1)*(S_F-1)+(S_F-1)*H(1)]*\hat{\Gamma}_{dd}\}(\mathbf{r}_1,\mathbf{r}_2)\ .\end{aligned} \tag{6.10}$$

Here, we use[1,2]

$$H(1)=-\frac{\hbar^2}{2m}\frac{1}{[\rho_1(\mathbf{r})]^{1/2}}\nabla\rho_1(\mathbf{r})\cdot\nabla\frac{1}{[\rho_1(\mathbf{r})]^{1/2}}\ . \tag{6.11}$$

Note that the lowest eigenstate of the one-body operator $H(1)$ is just the square root of the physical one-body density.

The remaining manipulations on the Euler-Lagrange equation (6.6) are similar to the ones performed for the Bose system.[1] We calculate the convolution product of (6.6) from the left with $(1-S_F*\hat{X}_{dd})$ and from the right with $(1-\hat{X}_{dd}*S_F)$. This leads to the final form of the fermion Euler-Lagrange equation

$$-[S_F^{-1}*H(1)*\hat{X}_{dd}+\hat{X}_{dd}*H(1)*S_F^{-1}-\hat{X}_{dd}*H(1)*\hat{X}_{dd}](\mathbf{r}_1,\mathbf{r}_2)=2\hat{V}_{p\text{-}h}(\mathbf{r}_1,\mathbf{r}_2)\ , \tag{6.12}$$

$$\hat{V}_{p\text{-}h}(\mathbf{r}_1,\mathbf{r}_2)=\hat{X}'_{dd}(\mathbf{r}_1,\mathbf{r}_2)-\tfrac{1}{4}[H(1)*\hat{X}_{dd}+\hat{X}_{dd}*H(1)](\mathbf{r}_1,\mathbf{r}_2)\ . \tag{6.13}$$

[S_F^{-1} in Eq. (6.12) is the inverse of S_F in the sense of the convolution product (2.16)]. Finally we may use the Euler equation (6.12) to eliminate $X'_{dd}(\mathbf{r},\mathbf{r}')$ from $N'_{dd}(\mathbf{r},\mathbf{r}')$, and the FHNC equations (5.6) and (5.9) to express $u_2(\mathbf{r},\mathbf{r}')$ in terms of $\Gamma_{dd}(\mathbf{r},\mathbf{r})$ and $N_{dd}(\mathbf{r},\mathbf{r}')$. Thus we find

$$\hat{V}_{p\text{-}h}(\mathbf{r}_1,\mathbf{r}_2)=[\rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2)]^{1/2}\left[[1+\Gamma_{dd}(\mathbf{r}_1,\mathbf{r}_2)]v(|\mathbf{r}_1-\mathbf{r}_2|)+\frac{\hbar^2}{2m}[\,|\nabla_{r_1}[1+\Gamma_{dd}(\mathbf{r}_1,\mathbf{r}_2)]^{1/2}|^2+|\nabla_{r_2}[1+\Gamma_{dd}(\mathbf{r}_1,\mathbf{r}_2)]^{1/2}|^2]\right]$$

$$-\tfrac{1}{2}\Gamma_{dd}(\mathbf{r}_1,\mathbf{r}_2)[\hat{N}_{dd}*H(1)*S_F^{-1}+S_F^{-1}*H(1)*\hat{N}_{dd}+\hat{X}_{dd}*H(1)*\hat{X}_{dd}](\mathbf{r}_1,\mathbf{r}_2)\;. \tag{6.14}$$

Equations (6.12) and (6.14) together with the chain equation (5.7) form a closed set of equations for the determination of the required two-body quantities. It was shown in I that in a Bose system $V_{p\text{-}h}(\mathbf{r}_1,\mathbf{r}_2)$ is the particle-hole interaction. Some sacrifices have been made in the present case of Fermi statistics: the particle-hole interaction in a Fermi fluid is nonlocal. The variational wave function (1.1) with local correlation operators amounts, if no further approximations are made, to special spatial averagings of the nonlocalities.[6] The FHNC approximation spelled out here explicitly goes a step further by neglecting the nonlocal portions of the particle-hole interaction. Translating this into the language of conventional perturbation theory, the present level of FHNC is equivalent to the self-consistent summation of ring and ladder diagrams, but does not contain corrections to the particle-hole propagators or self-energy insertions.

VII. SUMMARY

We have formulated in this paper a theory of optimized variational wave functions for an inhomogeneous Fermi system. Our derivations were exact, within the Feenberg model (1.1) of the ground-state wave function, for the determination of the single-particle basis. In the treatment of the two-body equation we have restricted ourselves to the simplest implementation of the FHNC theory. This simplification is not mandatory;[16] we have resorted to that approximation for the sake of a compact notation as a starting point for numerical application until some practical experience is gained.

Through the manipulations in the preceding sections we have encountered a number of related problems: These were the choice of the single-particle basis, the determination of the one-body attenuation factor, and the appearance of reducible diagrams due to the nonconservation of linear momentum. We have succeeded in eliminating the reducible diagrams by an optimal choice of the single-particle basis. This optimal basis minimizes the energy expectation value in the space of *all* correlated wave functions of the Feenberg form (1.1). At the same time we have decoupled the remaining problem of determining the one- and two-body correlations: The two-body equation (6.12) has an acceptable solution for any single-particle basis. This is necessary in order to permit an iterative solution.

The two-body equation in the present formulation is hardly more complicated than the corresponding two-body equation for a Bose system. We anticipate therefore that the problem can be solved numerically for systems with a simple geometry, for example, films or droplets of ^{3}He atoms, metal films and surfaces, or for simple models of finite nuclei. We have in the present paper deliberately refrained from presenting numerical results since details of the implementation of the theory will be somewhat different for different systems. The electron gas in a metal film or a surface is probably the system that allows for the most straightforward application of the formalism.

The variational theory offers a number of significant advantages compared with conventional perturbative treatments: Conventionally, the calculation of correlation energies starts with the response function, obtains the static form factor by frequency integration, and calculates finally the correlation energy by coupling-constant integration.[19] To our knowledge, this procedure has not been solved in a satisfactory way for a metal surface; only partial results and asymptotic properties are known so far.[20–22] The equivalent of the RPA within the variational theory is obtained by approximating the particle-hole interaction (6.14) by the bare Coulomb potential. In other words, the first iteration of our theory yields the equivalent of the RPA. This "variational" RPA contains a collective approximation for the particle-hole propagator[23] which in bulk systems is known to be accurate within a few percent.[16] The iterations of the FHNC-EL equations build in the local screening. An important aspect of the theory will be the derivation of the one-body Hamiltonian appearing in the generalized Hartree-Fock equation (4.19). We expect that our approach can predict surface properties of metals with a typical accuracy on the percent level. Finally, we note that our theory provides pair-correlation functions and single-particle orbitals that can be used in a more accurate Monte Carlo calculation of ground-state properties.

The prospects of our theory for the surface of liquid ^{3}He are comparable to what we have obtained in I for the surface of ^{4}He films. The simplification of the FHNC equations to the lowest level is not very severe; the inclusion of a few higher-order diagrams can improve the accuracy.[17] The main problem in ^{3}He, as in ^{4}He, is that the elementary diagrams and three-body correlations are not negligible. A further complication in ^{3}He is that the collective particle-hole propagator generates an additional inaccuracy of the same order of magnitude as the neglect of elementary diagrams or three-body correlations. In order to treat the ^{3}He surface as accurately as the electron gas, one needs probably the combination of a Monte Carlo calculation with the optimized wave functions obtained within our theory, and some kind of correlated-basis-functions treatment of the propagator corrections.

It is more difficult to assess the prospects of applying the variational theory to a finite nucleus. It is not so much the change in geometry (a spherical one instead of a planar) that generates the complications even if explicit provision must be made for the center-of-mass motion.

The complications originate from the structure of the nuclear forces. It is essential to iterate self-consistently between the chains and the parallel connected diagrams. A number of suggestions to include an explicit state (spin, isospin, tensor) dependence in the correlation factor are reported in the literature.[24–28] One might expect that those theories that include systematically and parallel-connected diagrams[24–26] are suitable candidates for the generalization of the variational theory to finite nuclear systems, even though other choices[27,28] of the state-dependent correlation operators have a more desirable operator structure. Perturbative corrections within the theory of correlated basis functions will also be necessary in order to account for the fact that the variational wave functions approximate the particle-hole spectrum by an effective collective mode.[23]

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