Spin-dependent correlations in the ground state of liquid ³He

M. Viviani

Scuola Normale Superiore, piazza dei Cavalieri, I-56100 Pisa, Italy and Istituto Nazionale di Fisica Nucleare, piazza Torricelli 2, I-56100 Pisa, Italy

E. Buendia

Departamento de Fisica Moderna, Universidad de Granada, E-18073 Granada, Spain

S. Fantoni

Dipartimento di Fisica dell'Università degli Studi di Lecce, via Arnesano, I-73100 Lecce, Italy and Istituto Nazionale di Fisica Nucleare, piazza Torricelli 2, I-56100 Pisa, Italy

S. Rosati

Dipartimento di Fisica dell'Università degli Studi di Pisa, piazza Torricelli 2, I-56100 Pisa, Italy and Istituto Nazionale di Fisica Nucleare, piazza Torricelli 2, I-56100 Pisa, Italy (Received 14 August 1987)

The energy per particle, the sound velocity, and the static structure function of the ground state of normal-liquid ³He have been calculated by using the variational theory. Chain summation methods have been employed to evaluate the expectation value of a realistic Hamiltonian with a wave function including pair, triplet, spin-dependent and back-flow correlations. Semi-optimized functions have been used for the Jastrow and spin-dependent correlations. The important contribution from the elementary diagrams are appropriately taken into account by using the interpolating equation scheme. Spin-dependent correlations have been found to be important to get an equation of state which is in very close agreement with the experimental data.

I. INTRODUCTION

The understanding of the correlations among the constituents of a strongly interacting many-body system is a challenging problem which has been the object of extensive studies in recent years. Liquid ³He is particularly suited to study correlations under several respects. First of all, it is a dense system in which correlation effects are sizable. At the equilibrium density $\rho_0=0.277\sigma^{-3}$, with $\sigma=2.556$ Å, the average distance between two atoms is $r_0=(3/4\pi\rho_0)^{1/3}\approx 1\sigma$, which is approximately the distance at which the interparticle potential changes sign. The measured liquid structure function at the peak differs from that of an uncorrelated Fermi gas by ~25%.

In the second place, the interparticle interaction for both 4 He and 3 He liquids is well known. It is believed that the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i=1}^{N} \sum_{\substack{j=1\\(i,j)}}^{N} v(r_{ij}) , \qquad (1.1)$$

where $v(r_{ij})$ is the effective potential of Aziz *et al.*,¹ denoted as HFDHE2, provides a very good description of liquid helium. Recent results obtained for the ground state of liquid ⁴He by using the Green-function Monte Carlo (GFMC) method² are indeed in very good agreement with the experimental energies and the liquid structure functions over a wide range of densities. Liquid ³He is less dense than ⁴He; therefore, we expect the possible

contribution from three-body forces³ to be almost negligible.²

Finally, helium atoms, as constituents of liquid helium can be safely considered elementary particles (the first excited state of ³He atom is at ≈ 24 eV). This feature makes it possible to clear out the genuine many-body structural properties from the effects due to the excitations of its constituents.

The variational and the GFMC theories look the most powerful approaches to handle a Hamiltonian of the type given in Eq. (1.1), although both have not yet given completely satisfactory results for the ground state of liquid ³He. The GFMC technique still suffers from the occurrence of nodes in the ground-state wave function. The most reliable GFMC result for the ground-state energy is obtained within the fixed-node (FN) approximation⁴ and gives an upper bound of -2.37 ± 0.01 K,⁵ to be compared with the experimental value -2.47 K. On the other side, the variational method is faced with the problem of getting realistic trial wave functions, as well as with that of evaluating the expectation value of the Hamiltonian with sufficient accuracy. The best variational energy obtained so far⁶ is approximately -2.35 K at the equilibrium density with a wave function of the type

$$\Psi_{0} = F_{J}F_{T}S\left[\prod_{\substack{i,j=1\\(i < J)}}^{N}F_{SD}(i,j)\right]\Phi_{0}, \qquad (1.2)$$

where Φ_0 is the Fermi-gas wave function, F_J is the so-

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called Jastrow correlation operator given by

$$F_{J} = \prod_{\substack{i,j = 1 \\ (l < j)}}^{N} f_{2}(r_{ij}) .$$
(1.3)

 F_T is the triplet correlation operator defined as follows:

$$F_T = \prod_{\substack{i,j,k = 1 \\ (i < j < k)}}^N f_3(\mathbf{r}_{ij}, \mathbf{r}_{ik}) , \qquad (1.4)$$

and

$$\left(\prod_{\substack{i,j=1\\(i < j)}}^{N} F_{\text{SD}}(i,j)\right)$$

is the symmetrized product of state-dependent pair correlation operators, generating the Feynman-Cohen backflow,⁷ of the form

$$F_{\rm SD}(i,j) = f_k(i,j)$$

= exp{ $i\eta_B(r_{ij})\mathbf{r}_{ij} \cdot [\mathbf{\hat{K}}(i) - \mathbf{\hat{K}}(j)]$ }, (1.5)

with the operator $\widehat{\mathbf{K}}(i)$ acting on Φ_0 as shown by the following equation:

$$\widehat{\mathbf{K}}(i) \exp\left[i\sum_{j=1}^{N} \mathbf{k}_{\alpha_{j}} \cdot \mathbf{r}_{j}\right] = \mathbf{k}_{\alpha_{i}} \exp\left[i\sum_{j=1}^{N} \mathbf{k}_{\alpha_{j}} \cdot \mathbf{r}_{j}\right].$$
(1.6)

A pure Jastrow model, at the experimental equilibrium density ρ_0 , gives an upper bound of ≈ -1.3 K,^{6,8} which results from the sum of a kinetic energy of 13.2 K and a potential energy of -14.5 K. Triplet correlations $f_3(\mathbf{r}_{ii}, \mathbf{r}_{ik})$ are somewhat weaker than f_2 , but nevertheless quite important since they bring the saturation density of the system very close to the experimental value ρ_0 and lower the energy per particle at the equilibrium by ≈ 0.55 K (Refs. 6 and 9) with a quenching of the kineticenergy mean value of $\approx 5\%$. State-dependent correlations are then expected to lower the energy per particle of $\approx 0.5 - 0.6$ K, without appreciably modifying the saturation density and bring the energy per particle of the normal spin-unpolarized state of liquid ³He below that of the fully polarized phase.⁶ Unfortunately, state-dependent correlations cannot be treated at the same degree of accuracy as the Jastrow and triplets correlations, due to the noncommutativity of the operators $F_{SD}(i, j)$ among themselves. In the calculation of Ref. 6 the treatment of the backflow correlation $f_k(i,j)$ is the major source of uncertainties. Three-body backflow terms, neglected in that calculation, account for $\approx 0.1-0.2$ K (Ref. 10) to the energy per particle. Moreover, a more involved state dependence than the one given in Eq. (1.5) seems to be necessary in order to fully describe the ground state of liquid ³He. In Ref. 11 it has been found that the state dependence carried by the backflow correlations is not completely adequate to explain the effective mass of one ³He impurity in ⁴He.

Recently^{12,8} two accurate integral-equations methods, based on the hypernetted-chain (HNC) theory and on the "interpolating approximation" for the elementary diagrams, have been developed for Bose (HNC/ α) and Fer-

mi (FHNC/ α) liquids. They have been used to calculate the binding energy and the liquid structure function of Jastrow-plus-triplets (JT) models of both liquid ⁴He and liquid ³He, providing results which are in very good agreement with the available Monte Carlo calculations¹³ and with those obtained by using the "scaling approximation" (HNC/s and FHNC/s).^{14,6}

In this paper we generalize the FHNC/ α (interpolating-equation) method to treat a correlation operator containing state-dependent correlations. It is shown that for the JTB (Jastrow + three-body + back-flow) model defined by Eqs. (1.2)–(1.6) the FHNC/ α gives results which compare reasonably well with the corresponding FHNC/s estimates, especially at the saturation density. The state dependence of $F_{SD}(i,j)$ is here analyzed in greater detail than in previous variational calculations. ^{15–17} Spin-dependent correlations of the type

$$f_{\sigma}(i,j) = 1 + \eta_{\sigma}(\mathbf{r}_{ij})\boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{j}$$
(1.7)

are explicitly included in the trial wave function Ψ_0 . They are expected to play a significant role on the behavior of the single-particle excitations, ^{15–17} as well as on that of the spin density structure function. ^{18,19} An improved version of the FHNC/SOC (single-operator-chain) approximation, ²⁰ which includes the most important higher-order corrections, ²¹ has been used to evaluate the many-body contributions due to $f_{\sigma}(i, j)$.

It is found that a JTS model, with an optimized $f_2(r_{ij})$ and a semioptimized $\eta_{\sigma}(r_{ij})$, gives a binding energy of 2.31 K at the saturation density. There are some advantages in the JTS model over the JTB model connected with the calculation of the many-body contributions to the distribution functions and of the spin-density structure function.

If both spin-dependent and backflow correlations are included in F_{SD} and if higher-order corrections to the SOC/SOR (single-operator-chain-single-operator-ring) scheme as well as three-body backflow cluster terms are included in the calculation of $\langle H \rangle$ (JTSB3 approximation; Jastrow + triplet + spin-dependent correlations + three-body backflow), the value -2.47 K is obtained for the ground-state energy at saturation density ρ_0 . The kinetic-energy expectation value is found to be $\langle T \rangle = 11.8$ K, which differs from the corresponding GFMC-FN (fixed-node) evaluation of Ref. 5 of ≈ 0.5 K. The reason for such a discrepancy is not well understood at present. It should be noticed that there is a large cancellation between potential and kinetic energies and, as a consequence, a variational calculation giving a good upper bound for the total energy may still miss details of the wave function Ψ_0 which are relevant to $\langle T \rangle$. Moreover, it is an interesting problem to fully recognize the differences between the variational and the GFMC treatments as far as the long-range part of Ψ_0 is concerned. The sound velocity and the liquid structure function are also found to be in very good agreement with the experimental data, showing on one side that spin correlations are important to get a realistic ground-state trial wave function and, on the other side, that possible three-body interactions to be added to the Hamiltonian (1.1) have

negligible effects on the static properties of liquid ³He.

The FHNC/ α method used in the calculation of the distribution functions of a JSTB wave function is outlined in Sec. II. The expression of the energy expectation value and of the liquid structure function are given in Sec. III. The results are presented and discussed in Sec. IV.

II. FHNC/ α METHOD

Very accurate evaluations of the two-body distribution function $g(r_{ij})$ for JT wave functions are obtained by using the FHNC/ α theory.^{12,8,9} If more involved trial wave functions of the JTSB type, given by Eq. (1.2) with

$$F_{\rm SD} = f_k(i,j) f_\sigma(i,j) \tag{2.1}$$

are employed, one has also to include the important many-body cluster terms containing backflow and spin correlations.

The single-operator-chain (SOC) approximation has been widely used in nuclear-matter calculations and in that case it is believed to furnish reliable results, mainly because state-dependent correlations are weaker than central correlations. Here also, one has $\eta_{\sigma}(r_{ij}) \ll 1$, therefore it is plausible that FHNC/SOC will be a good approximation for a JTS model wave function. Higherorder cluster terms of the type suggested in Ref. 21 and discussed in Appendix A provide for very small corrections to the energy expectation value.

Backflow correlations are treated as in Ref. 6. The inclusion of spin correlations in F_{SD} allows for keeping a backflow correlation $\eta_B(r_{ij})$ which is even weaker than that in Ref. 6, therefore the treatment used there is expected to be more justified in the present calculations.

Full derivations of the FHNC/SOC approximation, the FHNC/ α method for the JT model, and the approximation to sum cluster terms with backflow correlations can be found in the original paper.^{20,6,8,9} Here, we limit ourselves to combining the above treatments in order to evaluate the energy expectation value and the liquid structure function for JTSB model wave function at the best possible accuracy allowed by the present many-body technology.

The sum of chain diagrams, in the FHNC/SOC approximation, is given by the following nodal operators²⁰

$$\hat{\mathbf{N}}_{mn}(i,j) = N_{mn}^c + N_{mn}^\sigma \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j , \qquad (2.2)$$

where mn = dd, de, ee, and cc denote terms in which neither *i* nor *j* is exchanged, in which only *j* is exchanged, in which both *i* and *j* are separately exchanged, and in which both *i* and *j* belong to the same permutation loop, respectively. The function $N_{mn}^c(r_{ij})$ sums chain diagrams built up with central links only, namely Jastrow, triplets,



FIG. 1. Examples of diagrams contributing to g(r) and included in the present FHNC/ α scheme. Dashed, zig-zag, wavy lines represent $f_2^2 - 1$, η_B , and η_σ correlations, respectively. Shaded triangles correspond to triplet correlations $f_3^2 - 1$ and oriented lines to exchange correlations.

and backflow correlations, whereas $N_{mn}^{\sigma}(r_{ij})$ sums chain diagrams where each link contains only one η_{σ} correlation and may have additional central dressing. For instance, Figs. 1(a) and 1(c) contribute to N_{dd}^c , Fig. 1(b) to N_{de}^c , Fig. 1(d) to N_{dd}^{σ} , and Figs. 1(e) and 1(f) to N_{de}^{σ} . The central terms of the nodal operators are given by

$$N_{mn}^{c}(r_{ij}) = \rho \int d^{3}r_{k} \sum_{l,l'} \theta_{ll'}[g_{nl'}^{c}(r_{ik}) - \delta_{nl',dd}] \times [g_{ml}^{c}(r_{kj}) - N_{ml}^{c}(r_{kj}) - \delta_{ml,dd}],$$
(2.3)

where mn = dd, de, ee and l(l') is d or e,

$$\theta_{ll'} = (1 + \delta_{ll',dd})(1 + \delta_{ll',de})(1 + \delta_{ll',ed}) - 1 , \qquad (2.4)$$

and $\delta_{ll',mn}$ is 1 or 0 whether ll' = mn or not. The function N_{cc}^c is given by

$$N_{cc}^{c}(r_{ij}) = \rho \int d^{3}r_{k} \left[\left[g_{cc}^{c}(r_{ik}) + 3M_{e}N_{ca}^{\sigma}(r_{ik}) f_{2}^{2}(r_{ik}) h^{c}(r_{ik}) \right] \left[g_{cc}^{c}(r_{kj}) - N_{cc}^{c}(r_{kj}) + l(k_{F}r_{kj})/\nu \right] \\ + \left\{ 3M_{e}N_{cb}^{\sigma}(r_{ik}) \left[f_{2}^{2}(r_{ik}) h^{c}(r_{ik}) - 1 \right] \right\} g_{cc}^{c}(r_{kj}) \right]$$

$$(2.5)$$

The Slater function

$$l(x_{ij}) = 3[\sin(x_{ij}) - x_{ij}\cos(x_{ij})]/x_{ij}^{3}, \qquad (2.6)$$

with

$$x_{ij} = k_F t(r_{ij}) = k_F r_{ij} [1 + 2\eta_B(r_{ij}) + 2Z(r_{ij})], \qquad (2.7)$$

sums both the uncorrelated and backflow-correlated exchange links⁶ [in Eq. (2.5) the subtraction of the function $-l(k_F r_{jk})/\nu$ avoids the inclusion of chains with more than one uncorrelated exchange link]. The function $Z(r_{ij})$ includes the three-body dressed cluster terms of the type *dd* containing one backflow link $\eta_B(r_{ij})$ [see Fig. 1(g)]. In the case of the JTS model $\eta_B = Z = 0$ gives the standard value $x_{ij} = k_F r_{ij}$.

The functions $g_{mn}^c(r_{ij})$ sum all the diagrams of type mn, therefore also elementary terms should be included in their calculation. Following the interpolating procedure of Ref. 8 we get for $g_{mn}^c(r_{ij})$ the following expression:

$$g_{dd}^{c}(r_{ij}) = f_{2}^{2}(r_{ij})h^{c}(r_{ij}) + g_{dd}^{\text{SOR}}(r_{ij}) , \qquad (2.8)$$

$$g_{de}^{c}(r_{ij}) = f_{2}^{2}(r_{ij})h_{M}^{c}(r_{ij})T_{de}(r_{ij}) + g_{de}^{SOR}(r_{ij}) , \qquad (2.9)$$

$$g_{ee}^{c}(r_{ij}) = f_{2}^{2}(r_{ij})(h_{M}^{c}(r_{ij}) \{ T_{ee}(r_{ij}) + 2l[k_{F}t(r_{ij})]T_{cc}(r_{ij}) + \alpha(r_{ij})[T_{de}^{2}(r_{ij}) - \nu T_{cc}^{2}(r_{ij})] \} - h^{c}(r_{ij})l^{2}[k_{F}t(r_{ij})]/\nu) + g_{ee}^{\text{SOR}}(r_{ij}) , \qquad (2.10)$$

$$g_{cc}^{c}(r_{ij}) = f_{2}^{2}(r_{ij}) \{h_{M}^{c}(r_{ij})T_{cc}(r_{ij}) - h^{c}(r_{ij})l[k_{F}t(r_{ij})]/\nu\}, \qquad (2.11)$$

where

$$h_{\mathcal{M}}^{c}(r_{ij}) = \exp[\alpha(r_{ij})N_{dd}^{c}(r_{ij}) + C_{dd}(r_{ij}) + E_{dd}^{t}(r_{ij})], \qquad (2.12)$$

$$h^{c}(r_{ij}) = \left[\frac{\exp[\alpha(r_{ij})N_{dd}^{c}(r_{ij})] - 1}{\alpha(r_{ij})} + 1\right] \exp[C_{dd}(r_{ij}) + E_{dd}^{t}(r_{ij})], \qquad (2.13)$$

$$T_{mn}(r_{ij}) = N_{mn}^c(r_{ij}) + C_{mn}(r_{ij}) + D_{mn}(r_{ij}) \quad (mn \neq dd) .$$
(2.14)

The functions $C_{mn}(r_{ij})$ are obtained by integrating the triplet correlations $f_3^2(\mathbf{r}_{ij},\mathbf{r}_{ik})$, dressed with two-body bounds g_{mn} , on the coordinate \mathbf{r}_k . For instance, the link between particle l and particle m in Fig. 1(b) is summed in $C_{de}(r_{lm})$. Similarly, $\mathbf{Z}(r_{ij})$ and $D_{mn\neq dd}(r_{ij})$ sum all dressed three-body elements linear in η_B . Contributions of order η_B^2 are not treated exactly by the above equations. The expression of C_{mn} , \mathbf{Z} , and D_{mn} are given in Ref. 6 and are not reported here.

The function $g_{mn}^{SOR}(r_{ij})$ sum the single-operator ring (SOR) diagrams, ²⁰ like, e.g., Fig. 1(h), and they can be easily calculated by using Eqs. (6.34)–(6.36) of Ref. 20, with the result

$$g_{dd}^{\text{SOR}}(r_{ij}) = 3f_2^2(r_{ij})M_d^2 h^c(r_{ij}) [\eta_\sigma^2(r_{ij}) + h_M^\sigma(r_{ij})N_{dd}^\sigma(r_{ij})] , \qquad (2.15)$$

$$g_{de}^{\text{SOR}}(r_{ij}) = 3f_2^2(r_{ij})M_dM_e\{h_M^c(r_{ij})[\eta_\sigma^2(r_{ij}) + h_M^\sigma(r_{ij})N_{dd}^\sigma(r_{ij})]T_{de}(r_{ij}) + h^c(r_{ij})h^\sigma(r_{ij})N_{de}^\sigma\},$$
(2.16)

$$g_{ee}^{\text{SOR}}(r_{ij}) = 3f_{2}^{2}(r_{ij})M_{e}^{2}(h_{M}^{c}(r_{ij})[\eta_{\sigma}^{2}(r_{ij}) + h_{M}^{\sigma}(r_{ij})N_{dd}^{\sigma}(r_{ij})][T_{ee}(r_{ij}) + \alpha(r_{ij})T_{de}^{2}(r_{ij})]$$

$$+ h^{c}(r_{ij})h^{\sigma}(r_{ij})\{N_{ee}^{\sigma}(r_{ij}) - l^{2}[k_{F}t(r_{ij})]/\nu\}$$

$$+ h_{M}^{c}(r_{ij})h^{\sigma}(r_{ij})\{2N_{de}^{\sigma}(r_{ij}) + 2l[k_{F}t(r_{ij})]T_{cc}(r_{ij}) - \alpha(R_{ij})\nu T_{cc}^{2}(r_{ij})\}$$

$$+ h^{c}(r_{ij})\{N_{de}^{\sigma^{2}}(r_{ij}) + 2N_{cc}^{\sigma}l[k_{F}t(r_{ij})]/M_{e}\} - h_{M}^{c}(r_{ij})\nu T_{cc}(r_{ij})N_{cc}^{\sigma}(r_{ij})/M_{e}\}, \qquad (2.17)$$

where

$$h^{\sigma}(\mathbf{r}_{ij}) = 2\eta_{\sigma}(\mathbf{r}_{ij}) + N^{\sigma}_{dd}(\mathbf{r}_{ij}) ,$$
 (2.18)

$$h_{\mathcal{M}}^{\sigma}(r_{ii}) = 2\eta_{\sigma}(r_{ii}) + N_{dd}^{\sigma}(r_{ii})/2 , \qquad (2.19)$$

and the vertex corrections M_d and M_e are given in Appendix B. The function $g^{c}(r)$ given by

$$g^{c}(r) = g^{c}_{dd}(r) + 2g^{c}_{de}(r) + g^{c}_{ee}(r) , \qquad (2.20)$$

corresponds to the FHNC/ α approximation of the pair distribution function g(r). In the case of J or JT models of Ψ_0 , $g^{c}(r)$ approximates g(r) very well.⁸ If also

backflow and spin correlations are included in Ψ_0 , important many-body contributions are neglected in $g^c(r)$, like, e.g., SOC and three-body separable diagrams. A better approximation for the pair distribution, which includes the above diagrams will be discussed in the next section.

The function $E_{dd}^t(r)$ appearing in Eqs. (2.12) and (2.13) corresponds to the sum of the basic elementary diagrams of the type *dd* with at least one triplet correlation [see Fig. 1(i)]. The interpolating procedure automatically includes all the elementary diagrams which can be obtained by connecting two or more parallel chains N(r) with the two-body links $g_{mn}(r)$, via the relations^{12,8}

where $E^{(m+n)}(r)$ are the elementary diagrams obtained by connecting the m+n chains among themselves. In Ref. 8 it has been found that $\beta_{\alpha_1,\ldots,\alpha_n}=1$ is a good approximation, although the use of $\beta \approx 0$ for $(N_{de}^c)^2 (N_{dd}^c)^m$ and of $\beta=1$ for the all remaining cases seems to allow also the fulfillment of the condition S(0)=0. In this paper we keep all the β 's equal to unity and we extend the relations (2.21) to include possible parallel connections containing backflow and triplet correlations. More precisely [see Eq. (2.14)] we take

$$\prod_{i=1}^{n} T_{\alpha_{i}}(N_{dd}^{c})^{m} + E^{(m+n)} = \alpha(r)^{m+n-1} \prod_{i=1}^{n} T_{\alpha_{i}}(N_{dd}^{c})^{m} ,$$

$$(\alpha_{i} \neq dd) . \quad (2.22)$$

Diagrams $E_{dd}^{i}(r)$ are not of the type $E^{(m+n)}(r)$ and therefore they have to be explicitly included in the convolution equations. $E_{dd}^{i}(r)$ is here approximated by the sum of the four-point diagrams²² $E_{dd,4}^{i}(r)$ with the two-body links given by $g^{c}(r)$ of Eq. (2.20) calculated in Jastrow approximation. The reliability of this approximation is based on the property that $2g_{de}^{c}(r) + g_{ee}^{c}(r) \approx 0$ (Ref. 6) and that the pair distribution $g^{c}(r)$ does not change significantly under the inclusion of f_{3} , f_{σ} , and f_{k} .

The interpolating function $\alpha(r)$ is derived by considering the mass three-boson system described with a wave function of the Jastrow type with a short-range pair function f_s of the McMillan form. Then the interpolating function $\alpha(r)$ is taken to be⁸

$$\alpha(r) = 1 + \alpha_0 E_{\rm PY}(r) / N_{\rm PY}(r) , \qquad (2.23)$$

where α_0 is a constant parameter. $N_{PY}(r)$ is the nodal function satisfying the equation

$$N_{\rm PY}(r_{ij}) = \rho \int d^3 r_k [g_{\rm PY}(r_{ik}) - 1] \\ \times [g_{\rm PY}(r_{kj}) - N_{\rm PY}(r_{kj}) - 1], \qquad (2.24)$$

where $g_{PY}(r_{ij})$ is given by the Percus-Yevik approximation²³

$$g_{\rm PY}(r_{ij}) = f_s^2(r_{ij}) [1 + N_{\rm PY}(r_{ij})]$$
(2.25)

and $E_{PY}(r)$ is the Percus-Yevik prescription for the elementary diagrams, namely,

$$E_{PY}(r_{ij}) = -N_{PY}(r_{ij}) + \ln[1 + N_{PY}(r_{ij})] . \qquad (2.26)$$

The parameter α_0 is determined by requiring the compressibility consistency condition (CCC) for a classic fluid interacting through a potential $u(r) = v(r)/k_BT = -\ln f_s^2(r)$ and given by

$$1 + \rho \int d^{3}r[g(r) - 1] \int^{-1} = 1 + \frac{\rho}{3} \int d^{3}r \left[g(r) + \frac{\rho}{2} \frac{\partial g}{\partial \rho} \right] r u'(r) . \quad (2.27)$$

If, instead of the short-range f_s we have a pair correlation function $f_2(r)$ with a long-range tail, the above equation cannot be used anymore to get α_0 . In this case⁸ the parameter α_0 in Eq. (2.23) is calculated by requiring that the elementary functions $E_l(r)$ and $E_s(r)$ obtained with the long-range and short-range $f_2(r)$ be equal at the origin.

A typical behavior of the interpolating function $\alpha(r)$ is displayed in Fig. 2. The healing of $\alpha(r)$ to 1 guarantees that at large interparticle distances the FHNC/ α approximation merges into the FHNC/0 approximation which is a consequence of the fact that the elementary functions heal to zero much more rapidly than the nodal functions.

The spin terms of the nodal operators \hat{N}_{mn} defined by Eq. (2.2) are given by the following SOC equations:²⁰

$$N_{mn}^{\sigma}(r_{ij}) = \rho \int d^{3}r_{k} \sum_{l,l'} \theta_{ll'}^{\sigma}[g_{ml}^{\sigma}(r_{ik}) - N_{ml}^{\sigma}(r_{ik})]g_{l'n}^{\sigma}(r_{kj}) , \qquad (2.28)$$

where mn = dd, de and ee, l, l' = e, d and

$$\theta_{ll'}^{\sigma} = (1 + M_d \delta_{ll',dd})(1 + M_e \delta_{ll',de})(1 + M_e \delta_{ll',ed}) - 1 .$$
(2.29)

For the cyclic exchange chains one needs to distinguish two nodal functions $N_{ca}^{\sigma}(r_{ij})$ and $N_{cb}^{\sigma}(r_{ij})$, given by²⁰

$$N_{ca}^{\sigma}(r_{ij}) = \rho \int d^{3}r_{k} [g_{ca}^{\sigma}(r_{ik}) - N_{ca}^{\sigma}(r_{ik})] g_{cc}^{c}(r_{kj}) , \qquad (2.30)$$

$$N_{cb}^{\sigma}(r_{ij}) = \rho \int d^{3}r_{k} [g_{cc}^{c}(r_{ik}) - N_{cc}^{c}(r_{ik}) + l(k_{F}r_{ik})/\nu] g_{cb}^{\sigma}(r_{kj}) , \qquad (2.31)$$



FIG. 2. The interpolation function $\alpha(r)$ for the JTSB model at $\rho = \rho_0 (\alpha_0 = 0.96)$.

(2.24)

with

$$N_{cc}^{\sigma}(r_{ij}) = N_{ca}^{\sigma}(r_{ij}) + N_{cb}^{\sigma}(r_{ij}) .$$
(2.32)

The expression of the links g^{σ} are easily obtained by applying the interpolating procedure expressed by Eq. (2.22) to the SOC equations (6.18)-(6.20), (6.23), of Ref. 20, with the following results:

$$g_{dd}^{\sigma}(\mathbf{r}_{ij}) = f_2^2(\mathbf{r}_{ij})h^{c}(\mathbf{r}_{ij})h^{\sigma}(\mathbf{r}_{ij}) , \qquad (2.33)$$

$$g_{de}^{\sigma}(r_{ij}) = f_{2}^{2}(r_{ij}) [h^{\sigma}(r_{ij})h_{M}^{c}(r_{ij})T_{de}(r_{ij}) + h^{c}(r_{ij})N_{de}^{\sigma}(r_{ij})], \qquad (2.34)$$

$$g_{ee}^{\sigma}(r_{ij}) = f_{2}^{2}(r_{ij})(h^{\sigma}(r_{ij})h_{M}^{c}(r_{ij})[T_{ee}(r_{ij}) + \alpha(r_{ij})T_{de}^{2}(r_{ij})] - l^{2}[k_{F}t(r_{ij})]/\nu + h_{M}^{c}(r_{ij})\{2l[k_{F}t(r_{ij})]T_{cc}(r_{ij}) - \nu\alpha(r_{ij})T_{cc}^{2}(r_{ij})\} + h^{c}(r_{ij})N_{ee}^{\sigma}(r_{ij}) + 2h_{M}^{c}(r_{ij})N_{de}^{\sigma}(r_{ij})T_{de}(r_{ij})), \qquad (2.35)$$

$$g_{cx}^{\sigma}(r_{ij}) = f_2^2(r_{ij}) (M_e h^{\sigma}(r_{ij}) \{h_M^c(r_{ij}) T_{cc}(r_{ij}) - h^c(r_{ij}) l[k_F t(r_{ij})]/\nu] + h^c(r_{ij}) N_{cx}^{\sigma}(r_{ij})) \quad (cx = ca, cb) .$$
(2.36)

The three-particle distribution function, for a ground-state wave function Ψ_0 of a J or JT type, is given by

$$g_{3}(\mathbf{r}_{ij},\mathbf{r}_{ik}) = f_{3}^{2}(\mathbf{r}_{ij},\mathbf{r}_{ik}) \sum_{m,n,l,\dots} g_{mn}(\mathbf{r}_{ij}) g_{n',l}(\mathbf{r}_{jk}) g_{l',m'}(\mathbf{r}_{ki}) [1 + A_{m'',n'',l''}(\mathbf{r}_{ij},\mathbf{r}_{ik})] , \qquad (2.37)$$

where $A_{m'n''l''}$ is the sum of the Abe terms,²⁴ and the sum is extended to all the allowed FHNC combinations of the subscripts m, n, If state-dependent correlations are present in Ψ_0 nonfactorizable terms arise which should be added to the right-hand side of Eq. (2.37). We neglect these terms, and, moreover we approximate $g_{mn}(r_{ii})$ with $g_{mn}^{c}(r_{ii})$ and use the scaling approximation of Ref. 6 for the Abe functions, namely

$$A_{mnl \neq ddd}(\mathbf{r}_{ij}, \mathbf{r}_{ik}) = 0 , \qquad (2.38)$$

$$A_{ddd}(\mathbf{r}_{ij},\mathbf{r}_{ik}) = (1+s) A_{ddd,4}(\mathbf{r}_{ij},\mathbf{r}_{ik}) + A_{ddd,4}^{t}(\mathbf{r}_{ij},\mathbf{r}_{ik}) , \qquad (2.39)$$

where A_4 is the four-point Abe diagrams built with the link $g^{c}(r) - 1$ and A_{4}^{t} sums all those containing at least one triplet correlations. The scaling parameter s is here determined by solving the J model of the mass-threeboson system by using the HNC/ α scheme and requiring that the Jackson-Feenberg²⁵ (JF), and Pandharipande-Bethe²⁶ (PB) forms of the kinetic energies give the same result.⁶ It has been found important to consistently use

TABLE I. Comparison of FHNC/ α , FHNC/s, and MC (Monte Carlo) energies for the J, JT, JB, and JTB models with short-ranged correlations. The function $f_2(r_{ij})$, $f_k(i,j)$, and $f_3(\mathbf{r}_{ii},\mathbf{r}_{ik})$ and the MC estimates are taken from Ref. 13. The FHNC/s values are from Ref. 6. All the energies are in K.

Ψ_0	FHNC/α	FHNC/s	МС
J	-1.10	-1.08	-1.08 ± 0.03
JT	-1.62	-1.49	-1.61 ± 0.03
JB	-1.38		-1.55±0.04
JTB	- 1.98		-1.91 ± 0.03
	Ψ ₀ J JT JB JTB	$Ψ_0$ FHNC/α J -1.10 JT -1.62 JB -1.38 JTB -1.98	Ψ ₀ FHNC/ α FHNC/ s J -1.10 -1.08 JT -1.62 -1.49 JB -1.38 JTB

short-range or long-range pair correlations $f_2(r)$ for both Bose and Fermi systems.

Results of FHNC/ α calculations for J, JT, JB, and JTB models of Ψ_0 are compared in Table I with the MC¹³ and FHNC/s⁶ results, obtained in correspondence to shortranged $f_2(r)$ of the McMillan form. The contribution from back-flow correlations have been evaluated by using the same approximation as in Ref. 6, in which the threebody part of the back-flow kinetic energy terms has been neglected. There is an overall agreement among the three different approaches, with the FHNC/ α giving results which are slightly more close to MC estimates than the FHNC/s approximation.

III. CALCULATION OF THE ENERGY

The energy of the liquid can be calculated by using different forms of the kinetic energy. The Jastrow-Feenberg (JF) form^{25,27} is the one which looks the most adequate if triplet correlations are included in the wave function, since only the two- and the three-body distribution functions are involved in the energy calculation. Other commonly used forms, like the Pandharipande-Bethe (PB) form²⁶ and the Clark-Westhaus (CW) form^{28,29} require also the knowledge of the four- and five-body distribution functions.

The JF prescription provides the following expres $sions^{6,27}$ for the expectation value of the kinetic energy with the wave function Ψ_0 of Eq. (1.2):

$$T_{\rm JF}/N = T_F + T_B + T_{\Phi} + T_K , \qquad (3.1)$$

where T_F is the Fermi kinetic energy

$$T_F = \frac{3}{5} \frac{\hbar^2}{2m} k_F^2 , \qquad (3.2)$$

 T_{R} is the Boson-like term

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$$T_{B} = -\frac{\varkappa^{2}}{8m} \frac{\int d\tau \{\Phi_{0}^{*}[F^{+}(\nabla_{1}^{2}F) + (\nabla_{1}^{2}F^{+})F - 2(\nabla_{1}F^{+}) \cdot (\nabla_{1}F)]\Phi_{0}\}}{\int d\tau \Psi_{0}^{+}\Psi_{0}} , \qquad (3.3)$$

with F being the full correlation operator $F_J F_T S[\prod_{i < j=1}^N F_{SD}(i,j)]$ and T_{Φ} and T_K are given by

$$T_{\Phi} = \frac{\hbar^2}{8m} \frac{\int d\tau [(\nabla_1^2 \Phi_0^*) F^+ F \Phi_0 + 2(\nabla_1 \Phi_0^*) F^+ \cdot F(\nabla_1 \Phi_0) + \Phi_0^* F^+ F(\nabla_1^2 \Phi_0)]}{\int d\tau \Psi_0^+ \Psi_0} , \qquad (3.4)$$

$$T_{K} = -\frac{\hbar^{2}}{2m} \frac{\int d\tau [\Phi_{0}^{*}F^{+}(\nabla_{1}F)\cdot(\nabla_{1}\Phi_{0}) - (\nabla_{1}\Phi_{0}^{*})F^{+}\cdot(\nabla_{1}F)\Phi_{0}]}{\int d\tau \Psi_{0}^{+}\Psi_{0}}$$
(3.5)

The energy per particle can be written in the following form:

$$E_{\rm 1F}/N = T_F + W + W_{\Phi} + U + U_{\Phi} , \qquad (3.6)$$

where the W's and the U's correspond to the two-body and three-body energy terms, respectively. The approximation adopted to take into account state-dependent correlations consists on treating exactly the two-body cluster terms, adding to these the many-body cluster contribution in accordance with SOC and SOR approximation.²⁰ This implies that up to five operators may have one external point in common. Central correlations are included at any cluster order.

The W term is more conveniently separated into five pieces,

$$W = W_0 + W_s + W_c + W_{cs} + \Delta W$$
, (3.7)

where W_0 sums all the diagrams which have no operator chain connecting the two external points *i* and *j*, W_s corresponds to diagrams having a reducible SOR at either external points *i* or *j*, W_c is the sum of diagrams with one SOC, and W_{cs} sums diagrams with both one SOC and one SOR at *i* or *j*. Higher-order correlations to SOR and SOC approximations are included in ΔW , as discussed in Appendix A. Few examples of diagrams contributing to *W* are given in Fig. 3, where the black bubble between *i* and *j* generically denotes the interaction-type link

$$f_{2}(r_{ij})F_{SD}^{+}(i,j)H(i,j)F_{SD}(i,j)f_{2}(r_{ij})$$
.

The term W in Eq. (3.6) contains the expectation values of the potential and the two-body parts of T_B and T_K given by Eqs. (3.3) and (3.5), respectively. One easily finds that there are three different types of two-body operators $\hat{H}(mn)$, $\hat{B}_{de}(mn)$, and $\hat{B}_{cc}(mn)$ of the form

$$\hat{X}(mn) = \sum_{i,j=1,2} X^{ij}(mn) O^{i}(mn) O^{j}(mn) , \qquad (3.8)$$

with $O^{i}(mn)=1, \sigma_{m} \cdot \sigma_{n}$ for i=1,2 and they have to be dressed with central chains SOC and SOR. The operator $\hat{H}(mn)$ has the following components:

$$H^{ik} = f^i f^k v - \frac{\hbar^2}{4m} [f^i (\nabla^2 f^k) - (\nabla f^i) \cdot (\nabla f^k)], \quad (3.9)$$

where the f^{i} are defined by the equation

$$f_2(r_{mn})f_{\sigma}(r_{mn}) = \sum_{i=1,2} f^i(r_{mn})O^i(mn) , \qquad (3.10)$$

and therefore are given by

$$f^{1}(\mathbf{r}_{mn}) = f_{2}(\mathbf{r}_{mn}), \quad f^{2}(\mathbf{r}_{mn}) = f_{2}(\mathbf{r}_{mn})\eta_{\sigma}(\mathbf{r}_{mn}) \quad .$$
 (3.11)

The operator $\hat{H}(mn)$ is of the *dd* type, i.e., it gives rise to both a direct and an exchange term. The other two operators \hat{B}_{de} and \hat{B}_{cc} come from the kinetic energy operators acting directly on the backflow correlation $f_k(m,n)$ and \hat{B}_{de} cannot have any exchange on particle *n* whereas \hat{B}_{cc} is purely an exchange term. They are given by

$$B_{de}^{ik} = \frac{2\hbar^2 k_F^2}{5m} [r\eta'_B + 3\eta_B + r^2(\eta'_B)^2 + 2r\eta_B \eta'_B + 3\eta_B^2] f^i f^k , \qquad (3.12)$$

$$B_{cc}^{ik} = -\frac{\hbar^2}{m} (r\eta_B'' + 4\eta_B') f^i f^k l_p , \qquad (3.13)$$



FIG. 3. Examples of diagrams included in the energy calculation. (a) Belongs to W_0 , (c) to W_s , (b) and (e) to W_c , (d) to W_{cs} , and (f) to ΔW .

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with

$$l_p = \frac{\partial l(k_F t)}{\partial t} \quad . \tag{3.14}$$

By combining the interpolating procedure⁸ discussed in the previous section with the operator algebra of FHNC/SOC theory,²⁰ one gets the following expression for the $W_0 + W_s$ appearing in Eq. (3.7):

$$W_{0} + W_{s} = \frac{\rho}{2} \int d^{3}r \{ (H^{ii} + B^{ii}_{de}) [h^{c}(M^{i1i}_{d})^{2} + h^{c}_{M}M^{i1i}_{d}M^{i1i}_{e}T_{de}] + H^{ii}h^{c}_{M}M^{i1i}_{e}(T_{de}M^{i1i}_{d} + T_{ee}M^{i1i}_{e} + \alpha T^{2}_{de}M^{i1i}_{e}) \} A^{i}$$

$$+ \frac{\rho}{4} \int d^{3}r \{ [H^{ik}l(k_{F}t) + B^{ik}_{cc}] [-h^{c}l(k_{F}t)/\nu + h^{c}_{M}T_{cc}] + H^{ik}h^{c}_{M}T_{cc}[l(k_{F}t) - \nu\alpha T_{cc}] \} (M^{i1kmn}_{c})^{2}$$

$$\times (K^{nim}K^{1km} + K^{nkm}K^{i1m}) A^{m}, \qquad (3.15)$$

where a summation over the indices i, j, ... from 1 to 2 is implied and the matrix K^{ijk} is defined through the equation

$$O^{i}(mn)O^{j}(mn) = \sum_{k=1}^{2} K^{ijk}O^{k}(mn) , \qquad (3.16)$$

and its values are $K^{112} = K^{121} = K^{211} = 0$, $K^{111} = K^{122} = K^{212} = 1$, $K^{221} = 3$, and $K^{222} = -2$. The constant A^k , defined as $A^k = K^{kk1}$, results in $A^1 = 1$, $A^2 = 3$. The vertex corrections M_d^{ijk} , M_e^{ijk} , and M_c^{ijkmn} are given in Eqs. (B5) and (B6) of Appendix B.

The sum of the terms W_c and W_{cs} is more conveniently separated into four pieces depending on the exchange nature of the two-body operator existing between the two external points m and n, namely

$$W_{c} + W_{cs} = W_{x}(dd) + 2W_{x}(de) + W_{x}(ee) + W_{x}(cc) , \qquad (3.17)$$

where W_{cs} is approximated as in Ref. 20; therefore one has

$$W_{x}(dd) = \frac{\rho}{48} \int d^{3}r \ H^{ik} N_{dd}^{\sigma} [h^{c} + h_{M}^{c} (2T_{de} + \alpha T_{de}^{2} + T_{ee})] M_{d}^{2} (11K^{k2i} A^{i} + 10L^{k2i} + 9K^{ik2}) + \frac{\rho}{16} \int d^{3}r \ H^{ik} N_{dd}^{\sigma} \{ -h^{c} l^{2} (k_{F}t) / \nu + h_{M}^{c} [2l(k_{F}t)T_{cc} - \alpha \nu T_{cc}^{2}] \} M_{e}^{2} \times [\frac{1}{2} (K^{knm} L^{m2k} + K^{ikm} L^{n2m} + 3K^{knm} K^{mi2} + K^{knm} L^{m2k}) + \frac{1}{3} (4K^{n2m} K^{mik} A^{k} + K^{knm} L^{i2m} + K^{nim} L^{k2m})], \qquad (3.18)$$

$$W_{x}(de) = \frac{\rho}{4} \int d^{3}r (H^{ik}N_{de}^{\sigma} + B^{ik}_{de}N_{dd}^{\sigma})(h^{c} + h^{c}_{M}T_{de})M_{d}M_{e}(K^{k2i}A^{i} + L^{k2i}), \qquad (3.19)$$

$$W_{x}(ee) = \frac{\rho}{2} \int d^{3}r \, H^{ik} N_{ee}^{\sigma} h^{c} M_{d}^{2} K^{k2i} A^{i} , \qquad (3.20)$$

$$W_{x}(cc) = \frac{\rho}{2} \int d^{3}r \{ H^{ik}[h^{c}l(k_{F}t) - \nu h_{M}^{c}T_{cc}] + h^{c}B_{cc}^{ik}\} N_{ca}^{\sigma}M_{e}^{2}[K^{kim}(L^{n2m} + K^{n2m}A^{m}) + K^{nkm}L^{2im} + K^{imn}L^{k2m}] - 3\rho \int d^{3}r \{ H^{ik}[h^{c}l(k_{F}t) - \nu h_{M}^{c}T_{cc}] + h^{c}B_{cc}^{ik}\} (N_{ca}^{\sigma} - N_{cb}^{\sigma})M_{e}^{2}K^{nik}A^{k} .$$
(3.21)

The matrix L^{ijk} is defined in Ref. 20 and its values are $L^{112} = L^{121} = L^{211} = 0$, $L^{111} = 1$, $L^{122} = L^{212} = L^{221} = 3$, and $L^{222} = 6$. In preceding formulas we have taken for simplicity the same vertex factors M_d and M_e used in the SOC equations.

A completely similar procedure can be used to calculate W_{Φ} with the result

$$W_{\Phi} = W_{\Phi,0} + W_{\Phi,s} + W_{\Phi,x} , \qquad (3.22)$$

where

$$W_{\Phi,0} + W_{\Phi,s} = -\frac{\hbar^2}{4m\nu} \rho M_e^2 \int d^3r [f^i f^k (h^c \{ l(k_F t) \nabla_t^2 l(k_F t) + [\nabla_t l(k_F t)]^2 \} -\nu h_M^c T_{cc} \nabla_t^2 l(k_F t)) - 2\delta_{i1} \delta_{i1} N_{cc}^c \nabla^2 l(k_F r)] K^{nik} A^k , \qquad (3.23)$$

and

$$W_{\Phi,x} = W_{\Phi,x}(dd) + W_{\Phi,x}(cc) , \qquad (3.24)$$

with

$$W_{\Phi,x}(dd) = -\frac{\hbar^2}{32m} \rho M_e^2 \int d^3r \, f^i f^k N_{dd}^{\sigma} (h^c \{ l(k_F t) \nabla_t^2 l(k_F t) + [\nabla_t l(k_F t)]^2 \} - v h_M^c T_{cc} \nabla_t^2 l(k_F t)) \\ \times [\frac{1}{2} (K^{nim} L^{m2k} + 2K^{ikm} L^{n2m} + 3K^{knm} K^{mi2} + K^{knm} L^{m2i}) \\ + \frac{1}{3} (4K^{n2m} K^{mik} A^k + K^{knm} L^{i2m} + K^{nim} L^{k2m})], \qquad (3.25)$$

$$W_{\Phi,x}(cc) = \frac{\hbar^2}{2m} \rho M_e^2 \int d^3r \, f^i f^k h^c [\nabla_i l(k_F t)]^2 \{ \frac{1}{2} N_{ca}^{\sigma} [K^{kim} (L^{n2m} + K^{n2m} A^m) + K^{nkm} L^{2km} + K^{imn} L^{k2m}] - 3(N_{ca}^{\sigma} - N_{cb}^{\sigma}) K^{nik} A^k \} .$$
(3.26)

The term U in Eq. (3.6) corresponds to the kinetic energy due to triplet (U_T) and back-flow (U_K) correlations

$$U = U_T + U_K , \qquad (3.27)$$

where U_T comes from T_B of Eq. (3.3) and U_K from T_B and T_K . The term U_T , given by

$$U_T = -\frac{\hbar^2}{8m} \rho^2 \int d^3 r_{ij} \int d^3 r_{ik} \, g_3(\mathbf{r}_{ij}, \mathbf{r}_{ik}) \nabla_i^2 \ln f_3(\mathbf{r}_{ij}, \mathbf{r}_{ik}) \,, \qquad (3.28)$$

has been calculated by employing the three-body distribution function $g_3(\mathbf{r}_{ij}, \mathbf{r}_{ik})$ discussed in the previous section. In the approximation of Ref. 6 the term U_K has been completely neglected. Explicit expression for U_K can be found in Ref. 30.

The quantity U_{Φ} in Eq. (3.6) is a three-body kinetic energy part of T_{Φ} of Eq. (3.4). In practical cases it has been found to give a contribution to the energy which is less than 0.1%, and therefore it has been neglected.

An improved approximation to the distribution function g(r), with respect to $g^{c}(r)$ given in Eq. (2.20), can be easily obtained by using the equations derived for the energy expectation value, namely

$$g(r) = g_0(r) + g_s(r) + g_c(r) + g_{cs}(r) , \qquad (3.29)$$

where the terms $g_x(r)$ are obtained by the corresponding *W*'s given in Eqs. (3.15) and (3.17)–(3.21) by setting $B_{de} = B_{cc} = 0$ and $H^{ik} = f^i f^k$ and dropping out all the integrations. In such a way, Eq. (3.29) sums not only the diagrams included in $g^c(r)$, but also the SOC and separable diagrams. A more extensive discussion on the pair distribution function and on its spin-spin component is given elsewhere.³¹

IV. RESULTS

There are a few methods³²⁻³⁴ to calculate the optimum pair correlation function $f_2(r)$ for a J- (Jastrow) model wave function Ψ_0 . These methods differ among themselves mainly in the treatment of the elementary diagrams contributing to the expectation value of the Hamiltonian, and it is not completely clear which one furnishes the best $f_2(r)$ in a realistic case. Moreover, the generalization of those treatments to the case of a wave function Ψ_0 containing triplet and state-dependent correlations looks too complicated. Therefore we have preferred to use here a simpler method which provides a semioptimized pair correlation function with the proper long-range behavior

$$f_2(r \to \infty) = 1 - \operatorname{const}/r^2 . \tag{4.1}$$

The method consists in calculating the optimized f_2 for the mass three-boson system according to the HNC/ α version⁸ of the optimization process. One has to solve the following Euler equation

$$-\frac{\hbar^2}{m}\nabla^2 \sqrt{g(r)} + [v(r) + w_0(r) + w_E(r)]\sqrt{g(r)} = 0,$$
(4.2)

where $w_0(r)$ is the induced potential in HNC/0 approximation and $w_E(r)$ includes elementary diagrams contributions. The explicit expression of $w_0(r)$ and $w_E(r)$ are given in Ref. 8. The pair correlation function $f_2(r)$ extracted from the pair distribution function g(r), solution of Eq. (4.2), has proved to be remarkably adequate from the variational point of view.

The triplets correlation $f_3(\mathbf{r}_{ij}, \mathbf{r}_{ik})$ has been taken of the following form:⁶

$$f_3(\mathbf{r}_{ij},\mathbf{r}_{ik}) = \exp\left[\frac{1}{2}q\left(\mathbf{r}_{ij},\mathbf{r}_{ik}\right)\right], \qquad (4.3)$$

$$q(\mathbf{r}_{ij},\mathbf{r}_{ik}) = \sum_{\text{cycl}} \xi(\mathbf{r}_{ij}) \xi(\mathbf{r}_{ik}) \mathbf{r}_{ij} \cdot \mathbf{r}_{ik} , \qquad (4.4)$$

where \sum_{cycl} denotes the sum over the three permutations of the indices *ijk*, and the function $\xi(r)$ is given by

$$\xi(r) = \sqrt{\lambda_t} r \exp\left[-\frac{(r-r_t)^2}{w_t^2}\right].$$
(4.5)

A similar form has been considered for the back-flow correlation $\eta_B(r)$ also

$$\eta_B(r) = \lambda_b \exp\left[-\frac{(r-r_b)^2}{w_b^2}\right].$$
(4.6)

In Table II the FHNC/ α results are compared with the corresponding FHNC/s estimates.⁶ The values reported in Ref. 6 have been used for the parameter λ_x , r_x , and w_x (x = t, b) of the functions $\xi(r)$ and $\eta_B(r)$. The approximation of Ref. 6 has been used for the back-flow correlation terms. As in the case of the short-ranged pair correlation function, there is a good agreement between the

(2.07)

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$\rho(\sigma^{-3})$	Ψ_0	$lpha_0$	<i>(T)</i>	$\langle V \rangle$	E
0.237	J	1.13	10.58(10.71)	-12.12(-12.17)	-1.54(-1.46)
	JT	1.13	10.31(10.40)	-12.13(-12.19)	-1.82(-1.79)
	JTB	1.13	9.77(9.89)	-12.01(-12.11)	-2.24(-2.22)
0.277	J	0.93	13.25(13.48)	-14.55(-14.76)	-1.31(-1.28)
	JT	0.96	12.73(12.97)	-14.53(-14.80)	-1.80(-1.83)
	JTB	0.96	12.02(12.28)	-14.33(-14.50)	-2.31(-2.36)
0.301	J	0.85	14.93(15.22)	-15.92(-16.28)	-0.99(-1.06)
	JT	0.89	14.40(14.55)	-15.92(-16.33)	-1.61(-1.78)
	JTB	0.89	13.50(13.77)	-15.67(-16.12)	-2.17(-2.35)
0.330	J	0.77	17.18(17.69)	-17.57(-18.29)	-0.39(-0.60)
	JT	0.80	16.35(16.76)	-17.49(-18.31)	-1.15(-1.55)
	JTB	0.80	15.44(15.86)	-17.17(-18.03)	-1.73(-2.17)

TABLE II. Comparison of FHNC/ α and FHNC/s energies for the J, JT, and JTB models with long-ranged pair correlations. The FHNC/s values are those enclosed in parentheses and are taken from Ref. 6. All the energies are in K.

two variational schemes. For $\rho \leq \rho_0$ the results obtained for the total energy E compare very well, although the kinetic $\langle T \rangle$ and potential $\langle V \rangle$ energies separately do not agree as well. This is due to the different semioptimized pair correlation functions $f_2(r)$ adopted in the two calculations. Most of the differences in the two functions $f_2(r)$ are due to the fact that the induced potential $w_E(r)$ in Eq. (4.2) is neglected in the calculations of Ref. 6. Such differences do not seem relevant to evaluate the total energy, whereas they are important for quantities like $\langle T \rangle$, and the momentum distribution.^{8,9,35} A similar feature is more evident in the Bose case: if the HNC/ α scheme is used with a Jastrow factor derived from Eq. (4.2), where $w_E(r)$ is neglected, essentially the same results of the HNC/s scheme are obtained for $\langle T \rangle$, $\langle V \rangle$, and E, whereas if $w_E(r)$ in Eq. (4.2) is not neglected then the kinetic energy is appreciably reduced. For instance, at $\rho = 0.3648\sigma^{-3}$, $\langle T \rangle_{\alpha} = 14.69$ K, $\langle V \rangle_{\alpha} = -20.59$ K, and E = -5.90 K, whereas $\langle T \rangle_s = 15.25$ K, $\langle V \rangle_s = -21.19$ K, and E = -5.94 K.

As the value of the density ρ increases the scaling approximation for the elementary diagrams starts deviating from the interpolating equation method, and this explains most of the discrepancies shown in Table II for E at $\rho > \rho_0$.

The spin correlation function η_{σ} has been calculated by minimizing $W_0 + W_{\Phi,0}$, calculated by setting $g_{mn}^{\text{SOR}}(r) = 0$ in the FHNC/ α Eqs. (2.8)–(2.11), under the constraint that both $\eta_{\sigma}(r)$ and $[\eta_{\sigma}(r)]'$ heal to zero at some distance d_{σ} . This requirement is fulfilled by solving the following Euler equation:

$$-\frac{\hbar^2}{m}X(r)'' + [v(r) + w_{\sigma}(r) - \lambda]X(r) = w_c(r) , \quad (4.7)$$

with

$$\eta_{\sigma}(r) = X(r) / [rf_2(r)\sqrt{F_1(r)}]$$

and

$$w_{\sigma}(r) = -\frac{\hbar^2}{m} \frac{F_3(r)}{F_1(r)} - \frac{\hbar^2}{m} \left[-\frac{F_1(r)'}{4F_1(r)} - \frac{F_1(r)'}{2rF_1(r)} + \frac{[F_1(r)']^2}{4F_1(r)^2} \right],$$
(4.8)

$$w_{c}(r) = \frac{r}{4\sqrt{F_{1}(r)}} \left[\frac{\hbar^{2}}{m} [4F_{2}(r)\nabla^{2}f_{2}(r) + 4\nabla F_{2}(r)\cdot\nabla f_{2}(r) + f_{2}(r)\nabla^{2}F_{2}(r)] - 4F_{2}(r)v(r)f_{2}(r) - 2\frac{\hbar^{2}}{m}f_{2}(r)F_{3}(r) \right].$$
(4.9)

The functions $F_1(r)$, $F_2(r)$, and $F_3(r)$ are defined as

$$F_{2}(r) = -\frac{1}{v} \{ h^{c}(r) l [k_{F}t(r)] / 2 + h_{M}^{c}(r) T_{cc}(r) \}^{2}, \quad (4.10)$$

$$F_1(r) = g^c(r) / f_2^2(r) - v F_2(r)^2 , \qquad (4.11)$$

$$F_{3}(r) = h^{c}(r)(l[k_{F}t(r)]\nabla_{t}^{2}l[k_{F}t(r)] + \{\nabla_{t}l[k_{F}t(r)]\}^{2}), \qquad (4.12)$$

where the function $g^{c}(r)$ is defined in Eq. (2.20). The pa-

rameter λ is fixed by healing conditions. For a given choice of the function f_2 , f_3 , and η_B , the Euler equation (4.7) is solved in correspondence with different values of the healing distance d_{σ} to get the correlation function η_{σ} which minimizes the energy of the liquid. It has been found that the η_{σ} obtained in this manner provides better upper bounds of the energy than a three-parameter trial function of the same form as η_B of Eq. (4.6). The results obtained with a wave function Ψ_0 of the JTS type are given in Table III. The optimum values of λ_i , r_i , and w_i ,

TABLE III. Breakdown of the energy (in K) of the JTS models of liquid ³He as a function of the density ρ . α_0 is the parameter of the interpolating function.

$\rho(\sigma^{-3})$	0.237	0.277	0.301	0.330
α_0	1.13	0.96	0.89	0.80
T_F	2.71	3.00	3.17	3.38
Ŵ	-4.31	-4.49	-4.43	-4.08
W_{Φ}	-0.55	-0.66	-0.74	-0.85
U_T	-0.04	-0.15	-0.24	-0.41
ΔW	-0.008	-0.012	-0.02	-0.02
E_0	-1.95	-1.92	-1.69	-1.18
E_s	0.09	0.13	0.18	0.18
E_c	-0.26	-0.55	-0.82	-1.07
E_{cs}	0.02	0.04	0.08	0.09
$\langle T \rangle$	9.95	12.31	13.80	15.74
$\langle V \rangle$	-12.15	- 14.62	- 16.06	- 17.74
E	-2.19	-2.31	-2.26	- 1.99

obtained by minimizing the energy of the JT model of liquid ³He at $\rho = \rho_0$ result to be

$$\lambda_t = 0.75, r_t = 0.85\sigma, w_t = 0.45\sigma$$
, (4.13)

which coincide with those reported in Ref. 6. The dependence of these parameters on the density ρ has been found to be very weak and therefore the values given in Eq. (4.13) have been used at all the densities considered in the calculation. The quantities E_x with x=0, s, c, and cs reported in Table III are defined as

$$E_x = W_x + W_{\Phi,x} , (4.14)$$

and $\langle V \rangle$ and $\langle T \rangle$ denote the expectation value of the potential and kinetic energy, respectively.

The SOC contribution E_c to the energy results to be large and negative and the separable diagrams provide for a repulsive 10% correction. Typical values of the vertex correction $M_{x=d,e}$ are reported in Table IV.

Both the SOC-SOR contribution E_{cs} and the higherorder terms, summed in ΔW , result to be very small at all the densities, which strongly indicates that the approximation used in this calculation to take into account the many-body cluster terms with spin correlations is adequate.

A comparison of the results given in Tables II and III shows that the JTB and the JTS models give very similar equations of state for the liquid, with the JTS wave function being slightly preferable from the variational point of view. In fact corrections of $\approx 0.1-0.2$ K, due to the three-body back-flow term U_K should be added to the energies given in Table II.

The results of the variational calculation performed with the wave function Ψ_0 of the JTSB type, at the equilibrium density $\rho = \rho_0$, are reported in Table V as a function of the variational parameter λ_b . The calculation has been done by keeping the functions $f_2(r)$, $\xi(r)$, and $\eta_{\sigma}(r)$ as found for the JTS model wave function and by minimizing the energy with respect to the parameters r_b and w_b of $\eta_B(r)$. The best variational energy is obtained in

TABLE IV. Vertex corrections for the JTS model of liquid ³He.

$\rho(\sigma^{-3})$	0.237	0.277	0.301	0.330
M_d	1.101	1.100	1.100	1.090
M_{e}	0.969	0.964	0.954	0.930

correspondence to

$$\lambda_b = 0.15, r_b = 0.80\sigma, w_b = 0.375\sigma$$
 (4.15)

The contribution of U_K to the energy has been neglected in the minimization process. It has always been possible to find a minimum of the energy at all the densities considered. The various correlation functions obtained at $\rho = \rho_0$ are compared in Fig. 4, and the two-body distribution function g(r) corresponding to different choices of Ψ_0 is displayed in Fig. 5.

The energies per particle of the liquid obtained for different model wave functions at various values of the density are shown in Table VI. The energies E(JTSB2)correspond to the JTSB calculation discussed above and therefore they do not contain the contribution from U_{κ} . This has been estimated perturbatively, by calculating the expectation value of the three-body terms^{30, 10} of T_B and T_K of Eqs. (3.3) and (3.5), respectively, on the same wave function Ψ_0 obtained in the JTSB2 calculation. The superposition approximation [i.e., $A_{mnl} = 0$ in Eq. (2.37)] has been adopted for g_3 . The energies E(JTSB3) include such an estimation of U_K , which results to be positive and $\approx 10\%$ of the contribution to the energy from from the two-body back-flow term $U_2 = E(JTSB2) - E(JTS)$. The three-body terms of T_B and T_K coming from the Abe terms in g_3 are expected to give a negative contribution to the energy. We have not calculated them, but we have estimated them in the following way: We have repeated the energy minimization by computing the semioptimized η_{α} after having included the back-flow correlations in Ψ_0 . In this manner we get a different value of U_2 . We have then assumed U_K to be given by γU_2 and deter-

TABLE V. Breakdown of the energy (in K) of the JTSB model of ³He as a function of the variational parameter λ_b of the back-flow correlation η_B . The three-body back-flow term is neglected here. The Fermi kinetic energy $T_F = 3.00$ K. α_0 is the parameter of the interpolating function.

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λ _b	0	0.10	0.15	0.20
α_0	0.96	0.96	0.96	0.96
Ŵ	-4.49	-4.57	-4.55	-4.48
W _Φ	-0.66	-0.77	-0.81	-0.85
U_T	-0.15	-0.15	-0.15	-0.15
ΔŴ	-0.012	-0.010	-0.010	-0.009
$E_0 + E_s$	-1.79	-2.04	-2.09	-2.11
$\vec{E_c} + \vec{E_{cs}}$	-0.51	-0.46	-0.43	-0.38
$\langle T \rangle$	12.31	11.93	11.82	11.76
$\langle V \rangle$	-14.62	-14.43	- 14.34	- 14.25
E	-2.31	-2.50	-2.52	-2.49
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FIG. 4. The correlation functions f_2 (solid line), $10f_2\eta_B$ (dot-dashed line), and $10f_2\eta_\sigma$ (dashed line) for the JTSB model of liquid ³He at $\rho = \rho_0$.



FIG. 5. Comparison of pair distribution function g(r) for different models of the ground-state wave function Ψ_0 . Solid and dashed lines represent JT and JTSB model wave functions, respectively.

TABLE VI. Energies of liquid ³He for different models of the ground-state wave function Ψ_0 . Both JTSB2 and JTSB3 refer to the JTSB model. E(JTSB3) results include the estimate of the three-body back-flow term U_K . All the energies are in K.

$\rho(\sigma^{-3})$	<i>E</i> (J)	E(JT)	E(JTSB2)	E(JTSB3)
0.210	-1.53	-1.72	-2.22	-2.18
0.237	-1.54	-1.82	-2.39	-2.34
0.250	-1.49	-1.82	-2.44	-2.39
0.277	-1.31	-1.80	-2.52	-2.46
0.301	-1.00	-1.60	-2.43	-2.38
0.330	-0.38	-1.15	-2.24	-2.15

mined γ by equating the total energies obtained in the two different procedures. The results obtained are given in Table VII together with the calculated expectation values of the kinetic energy and the corresponding experimental data for $E(\rho)$. The data for $\rho < \rho_0$ are obtained by using an equation of state of the form

$$E(\rho) = E_0 + \sum_{i=1,5} a_i \left(\frac{\rho - \rho_0}{\rho_0} \right)^i, \qquad (4.16)$$

which fits³⁶ the measured sound-velocity data³⁷ at various pressure values of the liquid.

The energies E(JTSB) are very close to E(JTSB3) given in Table VI and in very good agreement with the experimental data. We have calculated the velocity of the sound c at equilibrium density from an equation of state of the form given in Eq. (4.16) with the coefficients a_i chosen so to reproduce the first five energies E(JTSB) of Table VII. The resulting estimate of the velocity of the sound is c=185 m/s which compares very well with the experimental results³⁶ $c_{expt}=182.90$ m/s. The liquid structure function S(k) displayed in Fig. 6 is also in remarkable agreement with the available experimental data.^{38,39}

The JTSB model of the ground state of liquid ³He results to be very realistic. Back-flow and spin correlations reproduce structural effects which are largely overlapping. In fact the gain in the energy due to the inclusion of both the correlations is lesser than the sum of the energy gains given by their separate inclusion. This can be explained by the fact that both correlations distinguish

TABLE VII. Comparison of the theoretical estimates of the energy per particle of liquid ³He with the experimental data. The data in brackets are extrapolated from the experimental equation of state (Ref. 37). All the energies are in K.

$\rho(\sigma^{-3})$	E(JTSB)	${E}_{ m expt}$
0.210	-2.19	(-2.16)
0.237	-2.35	(-2.35)
0.250	-2.40	(-2.41)
0.277	-2.47	-2.47
0.310	-2.39	-2.42
0.330	-2.17	-2.22



FIG. 6. Calculated liquid structure function S(k) compared with the experimental data at T=0.41 K of Ref. 38 (open triangles) and at T=0.76 K of Ref. 39 (solid triangles).

the L=0 from the L=1 relative angular momentum states of any two-particle system in the liquid. However, they have also independent effects which may be relevant in the study of the excited states of the liquid.³¹

The kinetic energies resulting from the present calculation are somewhat lesser than the corresponding vaule obtained by GFMC calculation. For instance, at $\rho = \rho_0$ we get $\langle T \rangle = 11.85$ K against the GFMC-FN (Ref. 5) estimate of 12.28 ± 0.04 K. The kinetic energy expectation value crucially depends on the details of the correlation operator and, for instance, a nonproper treatment of long-range behavior of the pair correlation function may lead to uncorrect estimates of $\langle T \rangle$. However, a correction to $\langle T \rangle$ of ≈ 3 K, as requested by the recently reported experimental value⁴⁰ appears to be too high.

The results obtained in the present calculation indicate that the HFDHE2 effective potential of Aziz *et al.*¹ provides a realistic description of liquid ³He and that fourbody correlations in Ψ_0 should have negligible effects at density values close to the experimental saturation density.

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APPENDIX A: MULTIPLE-OPERATOR CHAINS

In a FHNC/SOC calculation of the expectation value of the energy *E*, only diagrams with at most one singleoperator chain and with uncoupled single-operator rings are taken into account. The accuracy of such an approximation has been checked out in nuclear matter by Wiringa, ⁴¹ who computed the supposedly leading terms of the higher-order corrections to E and found them to be quite small in magnitude. However, in a dense system like liquid ³He higher-order corrections to the FHNC/SOC approximation could be of some relevance.

Let us briefly summarize the technique devised by Lagaris²¹ to calculate multiple-operator chain diagrams of the type shown in Fig. 7, in which each wavy line denotes the correlation $F=2f_2^2\eta_{\sigma}$ and the thick line corresponds to H^{11} [see Eq. (3.9)]. The operators $\sigma_i \cdot \sigma_j$ associated with each wavy line can come from either Ψ_0 in the expression $\langle \Psi_0 | H | \Psi_0 \rangle$. Therefore for a given diagram, one has various terms due to different partitions of the symmetrized products of $\sigma_i \cdot \sigma_j$ operators appearing on the right and on the left side of the Hamiltonian. For instance, for Fig. 7(a) one has the partition (0,4) with the symmetrized product of the four operators on the right of $H^{11}(i,j)$, namely

$$H^{11}(i,j)S[(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_l)(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_l)(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_m)(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_m)]/4!,$$

the partition (1,3) with one operator on the left and three on the right, etc. Due to the absence of operators in $H^{11}(i,j)$ each partition generates the same products of operators, therefore the generic diagrams $D_{k,2}$ having k chains made up with two wavy lines give rise to the following expression:



FIG. 7. Examples of multiple-operator chain diagrams included in the calculation of the energy expectation value (ΔW term).

$$D_{k,2}^{dd} = \rho^k \int d^3 r_1 \int \cdots \int d^3 r_k H^{11}(i,j) \prod_{n=1}^k F(r_{in}) F(r_{nj}) C_{ij}^{(k)} \left[S \left[\prod_{n=1}^k (\sigma_i \cdot \sigma_n) (\sigma_n \cdot \sigma_j) \right] \right] \alpha_k^{dd}, \qquad (A1)$$

where $C_{ii}^{(k)}(\cdots)$ means trace over the k external indices,

$$F(\mathbf{r}_{ij}) = 2f_2^2(\mathbf{r}_{ij})\eta_\sigma(\mathbf{r}_{ij}) , \qquad (A2)$$

and α_k^{dd} is a coefficient given by the sum of the weights of each partition divided by 2^{2k} . For instance $\alpha_2^{2d} = (2/4! + 2/3! + 1/4)/16 = 1/4!$. More generally one has²¹

$$C_{ij}^{(k)}\left[S\left(\prod_{n=1}^{k}(\boldsymbol{\sigma}_{i}\cdot\boldsymbol{\sigma}_{n})(\boldsymbol{\sigma}_{n}\cdot\boldsymbol{\sigma}_{j})\right)\right] = \begin{cases} (2k)!(k+1), & k \text{ even }, \\ \frac{1}{3}(2k)!(k+2)\boldsymbol{\sigma}_{i}\cdot\boldsymbol{\sigma}_{j}, & k \text{ odd }, \end{cases}$$
(A3)

$$\alpha_k^{dd} = \frac{1}{2^{2k}} \left[\sum_{\mu=0}^{2k} 1/\mu! (2k - \mu)! \right] = \frac{1}{(2k)!}, \quad k \ge 2.$$
(A4)

As a result, the sum of all the diagrams of the type $D_{k,2}^{dd}$ is given by

$$\sum_{k \ge 2} D_{k,2}^{dd} = \cosh(X_{ij}) + X_{ij} \sinh(X_{ij}) - 1 + [2\sinh(X_{ij}) + X_{ij} \cosh(X_{ij}) - 3X_{ij}] \frac{\sigma_i \cdot \sigma_j}{3} , \qquad (A5)$$

$$X_{ij} = \rho \int d^3 r_1 F(r_{i1}) F(r_{1j}) .$$
(A6)

A completely similar procedure can be followed in the case of diagrams of the type $D_{k,2}^{dd,exch}$ which have an exchange between *i* and *j*, like, e.g., Fig. 7(b). In fact, the exchange operator $P_{ij}^{\sigma} = (1 + \sigma_i \cdot \sigma_j)/2$ is always to the left of all the correlation operators in all the terms contributing to $D_{k,2}^{dd,exch}$, and one gets the following result:

$$\sum_{k\geq 2} D_{k,2}^{dd,\text{exch}} = -l(k_F r_{ij})^2 P_{ij}^{\sigma} \sum_{k\geq 2} D_{k,2}^{dd} .$$
 (A7)

It is easy to generalize the above procedure to calculate diagrams having operators chains built up with any number of operatorial links. The generic diagram of this type, $D_{k,\{\alpha\}}^{dd}$ has one chain with α_1 links, a second chain with α_2 links, etc., ..., and leads to an expression which differs from that of Eq. (A1) in the spatial part only. $\prod_{n=1}^{k} F(r_{in})F(r_{nj})$ is here substituted by the more involved chain structure $\prod_{n=1}^{k} F(r_{in_1}) \cdots F(r_{n_aj})$, whereas the $C_{ik}^{(k)}$ part and the weight α_k are given by

$$C_{ij}^{(k)} = \begin{cases} \left[\sum_{n=1}^{k} \alpha_n \right]! (k+1), & k \text{ even }, \\ \frac{1}{3} \left[\sum_{n=1}^{k} \alpha_n \right]! (k+2) \sigma_i \cdot \sigma_j, & k \text{ odd }, \end{cases}$$
(A8)

$$\alpha_k^{dd} = \frac{1}{\left(\sum_{n=1}^k \alpha_n\right)!}, \quad k \ge 2 , \qquad (A9)$$

and their product $C_{ij}^{(k)} \alpha_k^{dd}$ depends upon the number k of the parallel chains only. One can easily verify this result in the case of Fig. 7(c) by using the property that the C part of a generic product of the five $\sigma_i \cdot \sigma_j$ operators does not depend upon the position of the operator $\sigma_l \cdot \sigma_m$. The products $C_{ij}^{(k)} \alpha_k^{dd}$ has the same expression given above also in the case that an exchange operator P_{ij}^{σ} is associated with some of the links connecting internal points, like, e.g., in Fig. 7(d). The sum of all the multiple-chain diagrams $D_{k,\{\alpha\}}^{dd}$ of the type dd is then expressed as follows:

$$\sum_{k} D_{k,|\alpha|}^{dd} = \hat{L}_{dd}(i,j)$$
$$= L_{dd}^{c}(r_{ij}) + L_{dd}^{\sigma}(r_{ij}) \frac{\sigma_{i} \cdot \sigma_{j}}{3} , \qquad (A10)$$

where

$$L_{dd}^{c} = \cosh(N_{dd}^{\sigma}) + N_{dd}^{\sigma} \sinh(N_{dd}^{\sigma}) - 1 , \qquad (A11)$$

$$L_{dd}^{\sigma} = 2\sinh(N_{dd}^{\sigma}) + N_{dd}^{\sigma}\cosh(N_{dd}^{\sigma}) - 3N_{dd}^{\sigma} . \qquad (A12)$$

The function N_{dd}^{σ} takes also into account of some separable diagrams, like, e.g., Fig. 7(e), by means of proper vertex corrections. Their expressions, as discussed in Appendix B are derived for the case of separable diagrams having only one operator chain. The presence of more than one operator chain implies the occurrence of extra commutator terms. It turns out that these extra terms are generally reduced by a factor ≈ 5 with respect to the ordinary vertex corrections. Since the contribution is always quite small we have disregarded the mentioned extra corrections in this paper.

The discussed procedure can be used to calculate the multiple-chain diagrams of the type de, ee, and cc. The diagrams $D_{k,\{\alpha\}}^{de}$ having k-1 dd chains and one de chain [see Fig. 7(f)] furnish for the products $\alpha_k^{de}C_{ij}^{(k)}$ the same expression as those associated with the diagrams $D_{k,\{\alpha\}}^{dd}$ and given by Eqs. (A8) and (A9). There are two types of ee diagrams: those having two de chains [see Fig. 7(g)] are characterized by the weight

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$$\alpha_k^{ee1} C_{ij}^{(k)} = \begin{cases} (k+1) + \frac{2}{3} \frac{k+1}{k-1} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, & k \text{ even }, \\ \frac{k}{3} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, & k \text{ odd }, \end{cases}$$
(A13)

whereas the chains having one ee chain, like, e.g., Fig. 7(h), lead to the expression

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$$\alpha_k^{ee2} C_{ij}^{(k)} = \begin{cases} (k-1)\sigma_i \cdot \sigma_j, & k \text{ even }, \\ \frac{k}{3}(3-2\sigma_i \cdot \sigma_j), & k \text{ odd }. \end{cases}$$
(A14)

Finally, in the case of diagrams of the type cc, like Fig. 7(i) one gets the result

$$\alpha_k^{cc} C_{ij}^{(k)} = \begin{cases} (k+1)(1+\sigma_i \cdot \sigma_j), & k \text{ even }, \\ (k+2)(1-\sigma_i \cdot \sigma_j), & k \text{ odd }. \end{cases}$$
(A15)

It follows that the sum of all the multiple-chain diagrams $D^{\alpha\beta}$ with $\alpha\beta = de$, ee, and cc are given by

$$\hat{L}_{\alpha\beta}(i,j) = L^{c}_{\alpha\beta}(r_{ij}) + \frac{1}{3}\boldsymbol{\sigma}_{i} \cdot \boldsymbol{\sigma}_{j} L^{\sigma}_{\alpha\beta}(r_{ij}) , \qquad (A16)$$

where

$$L_{de}^{c} = N_{de}^{\sigma} \left[N_{dd}^{\sigma} \cosh(N_{dd}^{\sigma}) + 2\sinh(N_{dd}^{\sigma}) \right], \tag{A17}$$

$$L_{de}^{\sigma} = N_{de}^{\sigma} \left[N_{dd}^{\sigma} \sinh(N_{dd}^{\sigma}) + 3\cosh(N_{dd}^{\sigma}) - 3 \right], \qquad (A18)$$

$$L_{ee}^{c} = N_{ee}^{\sigma} [N_{dd}^{\sigma} \cosh(N_{dd}^{\sigma}) + 2\sinh(N_{dd}^{\sigma})] + (N_{de}^{\sigma})^{2} [3\cosh(N_{dd}^{\sigma}) + N_{dd}^{\sigma} \sinh(N_{dd}^{\sigma})] , \qquad (A19)$$

$$L_{ee}^{\sigma} = N_{ee}^{\sigma} \{ 3 [N_{dd}^{\sigma} \sinh(N_{dd}^{\sigma}) + \cosh(N_{dd}^{\sigma}) - 1] - [N_{dd}^{\sigma} \cosh(N_{dd}^{\sigma}) + 2\sinh(N_{dd}^{\sigma})] \}$$
(A 20)

$$+ (N_{de}^{0})^{2} \{ N_{dd}^{d} \cosh(N_{dd}^{0}) + 2 \sinh(N_{dd}^{0}) + [\cosh(N_{dd}^{0}) + 2 \sinh(N_{dd}^{0})/N_{dd}^{0}] \},$$
(A20)

$$L_{cc}^{c} = N_{cc}^{o} [N_{dd}^{o} \cosh(N_{dd}^{o}) + 2\sinh(N_{dd}^{o}) + N_{dd}^{o} \sinh(N_{dd}^{o}) + 3\cosh(N_{dd}^{o}) - 3], \qquad (A21)$$

$$L_{cc}^{\sigma} = N_{cc}^{\sigma} \{ 3[N_{dd}^{\sigma} \cosh(N_{dd}^{\sigma}) + 2\sinh(N_{dd}^{\sigma})] - [N_{dd}^{\sigma} \sinh(N_{dd}^{\sigma}) + 3\cosh(N_{dd}^{\sigma}) - 3] \} .$$
(A22)

As a consequence, the contribution ΔW to the energy expectation value due to the multiple-operator chain diagrams is given by

$$\Delta W = \Delta W(dd) + \Delta W(de) + \Delta W(ee) + \Delta W(cc) , \qquad (A23)$$

$$\Delta W(dd) = \frac{\rho}{2} \int d^3 r \, H^{11}([h^c + h_M^c(T_{ee} + 2T_{de} + \alpha T_{de}^2)]L_{dd}^c + \{-h^c l(k_F t)^2 / \nu + h_M^c [2l(k_f t)T_{cc} - \nu \alpha T_{cc}^2]\}(L_{dd}^c + L_{dd}^\sigma)), \qquad (A24)$$

$$\Delta W(de) = \rho \int d^3 r \, H^{11}(h^c + h_M^c T_{de}) L_{de}^c , \qquad (A25)$$

$$\Delta W(ee) = \frac{\rho}{2} \int d^3 r \, H^{11} h^c L_{ee}^c \,, \tag{A26}$$

$$\Delta W(cc) = \frac{\rho}{2} \int d^3 r \, H^{11}[h^c l(k_F t) - h^c_M v T_{cc}] L^c_{cc} \,. \tag{A27}$$

APPENDIX B: SEPARABLE DIAGRAMS

A separable diagram is a diagram which is constituted by two parts, connected by means of only one point called articulation point. The contribution of such diagrams can be included in the nodal function as a "vertex correction" as in Eq. (2.28);²⁰ that is, for a given point *i* of a diagram Γ all the separable diagrams having *i* as the articulation point are summed up with a numerical factor $M(x_{\Gamma}, y_{\Gamma})$ multiplying Γ . The variables x_{Γ} and y_{Γ} specify the diagrammatic elements of Γ which reach the articulation point *i* as in Ref. 20: $x_{\Gamma} = I$, f^2 , or *P* for an interaction line, a double wavy line or a chain, respectively; $y_{\Gamma} = e, e_{p}$, or d for an operatorial exchange loop, a central exchange loop, or a direct correlation, respectively.

In the present calculation we have taken into account separable parts of the SOR type having an articulation point in common with a SOC or SOR. Diagrams which have three or more SOR touching at the same point have been neglected. The resulting expression for M is

$$M(x_{\Gamma}, y_{\Gamma}) = 1 + D_{\sigma\sigma} \sum_{x_{S}, y_{S}} m(x_{\Gamma}, y_{\Gamma}, y_{S}, x_{S}) J(y_{\Gamma}, y_{S}, x_{S}) , \qquad (B1)$$

where $D_{\sigma\sigma} = -\frac{4}{3}$ and $m(x_{\Gamma}, y_{\Gamma}, y_{S}, x_{S})$ is a number between 0 and 1 coming from commutator contribution between Γ and the separable part S. $J(y_{\Gamma}, y_S, x_S)$ represents the contribution of S. x_S and y_S specify the diagrammatic elements coming at the articulation point from S: $y_S = e$, e_p , or d whereas $x_S = f^2$ or P. For example, if $y_{\Gamma} = e$, S cannot have an

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exchange loop at the articulation point and y_s is forced to be d. With the interpolating approximation we have

$$J(y_{\Gamma}, d, x_{S}) = 3\rho \int d^{3}r f_{2}^{2} X_{x_{S}} \{ [(M_{d}h^{c} + M_{e}h_{M}^{c}T_{de}) + \delta_{y_{\Gamma}, d}h_{M}^{c}(M_{d}T_{de} + M_{e}\alpha T_{de}^{2} + M_{e}T_{ee})](1 + N_{dd}^{\sigma}\delta_{x_{s}, P}) + (M_{e}h^{c} + M_{e}h_{M}^{c}T_{de}\delta_{y_{\Gamma}, d})N_{de}^{\sigma}\delta_{x_{s}, P} \},$$
(B2)

$$J(d,e,P) = 3\rho \int d^3r f_2^2 h^{\sigma} \{ -h^c l (k_F t)^2 / \nu + h_M^c [2l (k_F t) T_{cc} - \nu \alpha T_{cc}^2] \} M_e , \qquad (B3)$$

where h^c , h_M^c , and h_M^σ are defined in Eqs. (2.12), (2.13), and (2.19), respectively, and

$$X_{x_{S}} = \begin{cases} (\eta^{\sigma})^{2}, & x_{S} = f^{2}, \\ 2\eta^{\sigma}, & x_{S} = P. \end{cases}$$
(B4)

In the SOC equations (2.28) and in Eqs. (B2) and (B3) instead of using $M(x_{\Gamma}, y_{\Gamma})$ we have employed $M_d = \frac{1}{3} \sum_{x_{\Gamma}} M(x_{\Gamma}, d)$ when the correlations of Γ connected with the articulation point are only dynamical and $M_e = \frac{1}{5} \sum_{x_{\Gamma}} [M(x_{\Gamma}, e) + M(x_{\Gamma}, e_p)]$ when there is also an exchange loop [there are only five different M_e because $M(f^2, e) = 0$ in our approximation]. In fact the differences between the $M(x_{\Gamma}, d)$'s [or between the $M(x_{\Gamma}, e)$'s and $M(x_{\Gamma}, e_p)$'s] are small and in such a way all the equations look simpler.

When we have to calculate the expectation value of a two-body operator O_{mn} the vertex corrections in *m* and *n* are more involved, due to the presence of the many operators coming from $F^i(m,n)O^j(m,n)F^k(m,n)$ [here i=1 refers to the central component so $F^1=f_2$ and $O^1(m,n)=O(r_{mn})$, whereas i=2 refers to the operatorial component and $F^2=f_2\eta_{\sigma}$]. In that case we introduce a vertex correction in *m* and *n* which depends upon the indices *i*, *j*, and *k*:

$$M_{y}^{ijk} = 1 + \frac{1}{4}(D_{i2} + D_{j2} + D_{k2})J(y, d, f^{2}) + \frac{1}{24}(5D_{i2} + 3D_{j2} + 5D_{k2})J(y, d, P) + \delta_{y, d} \frac{1}{4}(D_{i2} + D_{k2})J(d, e, P) ,$$
(B5)

where $D_{22} = D_{\sigma\sigma}$, $D_{11} = D_{12} = D_{21} = 0$, and y = d, e. When an exchange loop is present between *m* and *n* there is another operator coming from the exchange operator $(1 + \sigma_m \cdot \sigma_n)/2$. Thus we have

$$M_{c}^{ijklm} = 1 + \frac{1}{24} (6D_{m2} + 3D_{j2} + 3D_{j2} + 2D_{i2} + 2D_{k2}) J(e, d, P) + \frac{1}{4} (D_{m2} + D_{j2} + D_{l2}) J(e, d, f^{2})$$
(B6)

which also depends upon the exchange operator's variable m.

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