

Spin-density fluctuations and the energy of liquid ³He

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We introduce spin-density fluctuations into the Slater-Jastrow trial wave function for liquid ³He using a spin-dependent correlation operator. The unpolarized ground-state energy is thereby lowered by 0.3 K and probably stabilized with respect to the polarized state. A crucial element in the calculation is the correct treatment of a substantial cancellation between direct and exchange contributions to the energy.

The Slater-Jastrow wave function

$$\psi = \exp\left\{\frac{1}{2} \sum_{i < j} u(i, j)\right\} |\phi\rangle, \tag{1}$$

with $u(i, j)$ depending only on relative separations, is widely used for the evaluation of the energy of normal liquid ³He. Monte Carlo calculations with this trial wave function¹ have shown, however, that the energy for the polarized liquid (all spins in $|\phi\rangle$ parallel) is about 0.4 (± 0.2) K lower than for the unpolarized liquid. Real liquid ³He does not show this ferromagnetism. Extrapolation from the measured susceptibility implies that the energy in the unpolarized phase should be the lower by a fraction of a degree K.

In this Communication we consider a wave function of the form (1) with a local, spin-dependent operator

$$u(i, j) = u^c(r_{ij}) + u^\sigma(r_{ij}) \vec{\sigma}_i \cdot \vec{\sigma}_j. \tag{2}$$

This operator introduces local spin-density fluctuations into the ground state which will lower the energy in the unpolarized phase, but will have no effect on the polarized phase (where spin and density fluctuations are equivalent).

We use the hypernetted chain (HNC) theory to evaluate an approximation to the energy and we determine $u^c(r)$ and $u^\sigma(r)$ by a free variation of this energy. We will show that the truncation of the energy expansion, particularly with regard to Pauli and exchange terms (even with $u^\sigma \equiv 0$) introduces uncertainties on the order of 0.2 K. We conclude tentatively that with the spin fluctuations the unpolarized phase has the lower energy at zero pressure, but that the polarized phase remains lower at higher pressures.

The mathematical problem is to evaluate the expectation value of the Hamiltonian

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

in the wave function (1) and (2). Apart from the added complication of the Slater determinant $|\phi\rangle$, the problem is equivalent to the evaluation of an expectation value for a Heisenberg ferromagnet.² The main difficulty here is that the spin operators in (2) do not commute amongst themselves. Formally, this can be overcome by assigning a fictitious time to each of the operators and introducing the Dyson time ordering or T product. The operators may then be assumed to commute within the T product. We have discussed this in detail elsewhere.³ For the present calculations we note that there are two classes of diagrams for which the noncommutivity of the spin operators is of no consequence. The first are the "ladder diagrams"^{3,4} which involve the repeated scattering of a pair of particles from the Fermi sea and the second are the ring or chain diagrams of single, spin-dependent correlations which control the possible accumulation of long-range spin correlations. In so far as we are concerned with the correct treatment of only these two classes of diagrams, the HNC theory follows exactly as for spin-independent correlations.⁷ We note that so far as these two classes of diagrams are concerned we can obtain identical results starting from the symmetrized product wave function of Pandharipande and Wiringa⁵ or the independent-pair wave function of Owen.⁶

The energy per particle is written as a sum over singlet (s) and triplet (t) states in this approximation as follows⁷

$$\frac{E}{N} = \frac{\hbar^2}{2m} \left[\frac{3k_F^2}{5} + \sum_{\alpha=s,t} \rho \int g^\alpha(r) V^{*\alpha}(r) d\vec{r} + T_{JF} \right], \tag{4a}$$

where

$$V^{*\alpha}(r) = -\frac{1}{4} \nabla^2 u^\alpha(r) + (m/\hbar^2) V(r), \tag{4b}$$

and

$$T_{JF} = \frac{1}{4} \int \tilde{\nabla}^2 (\langle \phi | e^u | \phi \rangle), \tag{4c}$$

and $\tilde{\nabla}^2$ acts only on the single-particle states in $|\phi\rangle$

and $\langle \phi |$. The functions $g^{s,t}(r)$ are the singlet and triplet state projections of the two-particle distribution function. The singlet and triplet projections are related to the central and spin components by

$$\begin{pmatrix} u^s \\ u^t \end{pmatrix} = \begin{pmatrix} 1 & -3 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} u^c \\ u^\sigma \end{pmatrix}. \quad (5)$$

$$u^\alpha(r) = \ln g_B^\alpha(r) - N^\alpha(r) - E_{dd}^\alpha(r), \quad \alpha = s, t, \quad (6a)$$

$$N^\beta(k) = g_B^\beta(k) \{ g_B^\beta(k) [1 + X_{ee}^\beta(k)] - [1 - X_{de}^\beta(k)]^2 + 1 \} / \{ 1 + [1 + X_{ee}^\beta(k)] g_B^\beta(k) \}, \quad \beta = c, \sigma, \quad (6b)$$

where X_{de} and X_{ee} are non-nodal subdiagrams in which one or both of the end points is exchanged. They are defined as functionals of g_B and evaluated in the approximation described in Ref. 7. E_{dd} is the sum of elementary diagrams in which neither of the end points is exchanged. It is set to zero. We note that the r -space equation separates into uncoupled singlet and triplet components and the k -space equation into central and spin components. We stress that for $u^\sigma \neq 0$ the spin component of Eq. (6b) is an approximation. It correctly describes chains of single u^σ correlations, but not chains built from the r -space parallel connection of two or more u^σ .⁵ We have assumed that these are negligible and it is more convenient to include them with incorrect coefficients, rather than to write equations which explicitly exclude them.

The calculation of the energy requires the components of the full distribution function $g^\alpha(r)$. These can be expressed as a sum of terms in g_B^α and particle exchanges.⁷ The leading terms in this expansion are shown in Fig. 1, where the dashed lines represent a renormalized correlation factor $g_B^\alpha - 1$ and the directed lines represent exchanges from the Slater determinant. We have extracted a factor of $g_B^\alpha(r)$ in order to cancel the repulsive core of the interaction. Those terms in which the two external points are within the same loop of exchange lines are called exchange terms and those in which they are in disjoint loops are direct terms. We find numerically that there is a substantial cancellation between direct and exchange terms involving the same number of renormalized correlation lines. In order to maintain this cancellation we will classify the terms according to the number of renormalized correlation lines which they contain. Diagrams (a) and (b) are first order, diagrams (c) and (d) are all of the second-order direct graphs, and (e) and (f) are the corresponding exchange graphs. Diagrams (c) to (h) are "ladder" diagrams, they do not mix singlet and triplet components of g_B and we evaluate them correctly. Diagram (i) is a nonladder term and mixes the singlet and triplet components of g_B . Maintaining the cancellation between direct and exchange graphs in this

To evaluate the energy we first eliminate the Jastrow correlation factors $u^\alpha(r)$ in favor of a renormalized correlation factor $g_B^\alpha(r)$. This factor is that contribution to the two-particle distribution function in which neither of the two end points is exchanged.⁷ This is accomplished explicitly by the HNC equations^{7,8}

expansion is an important aspect to the calculation and applies to both spin-independent and spin-dependent correlations. We expect, moreover, that the truncation of this expansion for g in terms of g_B is the main source of error in our calculation, and we use it to estimate the uncertainty in our results. This classification is similar to the Wu-Feenberg⁹ expansion of statistical correlations, although not identical, since our renormalized correlation function g_B already contains some statistical effects through X_{de} and X_{ee} .

The quantity T_{JF} may be expanded in powers of $g_B - 1$ in a similar way.⁷ We define the order of a contribution to T_{JF} to be equal to the number of dynamical correlation lines. This is consistent with

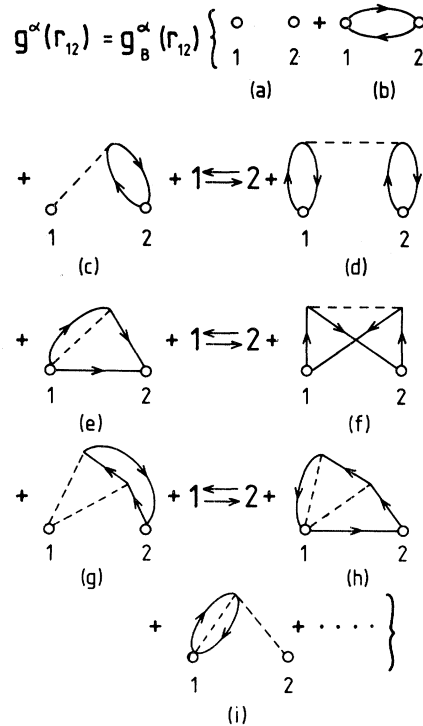


FIG. 1. Some diagrams in the expansion of $g(r)$ in terms of the dynamical correlation $g_B - 1$ (dashed line).

the classification given above when $g(r)$ is combined with V^* of (4b) to give an energy.

We have described the Euler-Lagrange equations for determining the optimal correlation functions for spin-independent correlations in Ref. 7. In the present case the equations are identical to Eqs. (4.1)–(4.3) of Ref. 7 except that all quantities and equations develop two components, either singlet and triplet for r -space equations or central and spin for k -space equations. The Euler-Lagrange equations are conveniently written as two-body scattering equations in singlet and triplet states as follows

$$\frac{-\hbar^2 \nabla^2 g_B^\alpha(r)^{1/2}}{m} + V(r) g_B^\alpha(r)^{1/2} + \rho \int S_F(|\vec{r} - \vec{r}'|) V(r') g_B^\alpha(r')^{1/2} d\vec{r}' = D^\alpha(r) \quad (7)$$

S_F is the two-particle distribution function for a noninteracting Fermi gas. It appears as a state-averaged Pauli operator and ensures the healing of g_B^α as $1 + O(r^{-2})$ for large r .⁷ The term $D^\alpha(r)$ represents the contributions due to scattering in exchange states and all higher-order terms. The exchange terms have opposite signs in singlet and triplet states and it is this difference which generates the spin correlations.

We have solved the Euler-Lagrange equations for the correlation functions and evaluated the energy using both spin-independent ($u^\sigma \equiv 0$) and spin-dependent correlations in both the polarized and unpolarized phases. Table I shows the energies at a

density of 0.016 \AA^{-3} . E_d and E_e are the contributions to the energy from the direct and exchange parts of $g(r)$ and the order refers to the classification according to the number of correlation lines as discussed above. The third-order contribution includes only diagrams (g) and (h) of Fig. 1.¹⁰ The penultimate column gives the total energy through the described order and the final column gives the Monte Carlo energies.¹

For the polarized phase the cancellation between direct and exchange diagrams beyond first order is almost complete and the net contribution in any order is dominated by T_{JF} . This cancellation is also evident for the unpolarized phase although it is not complete because only half of the particle pairs are exchanged. A FHNC resummation of this expansion will include the third-order exchange diagram (h) but not its direct partner (g). This has led to an overestimate of the difference in energy between the polarized and unpolarized phases.¹¹ We obtain a rough estimate of the uncertainty introduced by the truncation of this expansion by comparing the first- and second-order terms. These error estimates are given in Table I with the second-order energy.

Figure 2 shows our second-order energies for a range of densities in both the polarized (dashed line) and unpolarized phases together with some Monte Carlo results of Ref. 1. The error bars on our calculation are again obtained by comparing the first- and second-order contributions.

There remain two possible sources of error in our calculation. The first is the approximation of setting

TABLE I. Calculated energies (in K) at $\rho = 0.016 \text{ \AA}^{-3}$ for the polarized and unpolarized phases with spin-independent ($u^\sigma \equiv 0$) and spin-dependent ($u^\sigma \neq 0$) correlations. E_d and E_e are direct and exchange contributions from the described order, E is the total energy through the described order, and E_{MC} are from Monte Carlo calculations (Ref. 1). The order describes the number of renormalized correlation lines in the energy evaluation and does not apply to E_{MC} .

Order	E_d	E_e	T_{JF}	E	E_{MC}
Polarized					
Fermi				4.7	
1	-3.3	-1.3	-0.8	-0.7	
2	1.2	-1.1	-0.4	-1.0(±0.3)	-1.3(±0.2)
3 ^a	0.9	-1.0			
Unpolarized ($u^\sigma \equiv 0$)					
Fermi				2.9	
1	-2.8	-0.8	-0.4	-1.1	
2	0.8	-0.5	-0.1	-0.9(±0.2)	-0.9(±0.2)
3 ^a	0.5	-0.3			
Unpolarized ($u^\sigma \neq 0$)					
Fermi				2.9	
1	-2.8	-1.2	-0.4	-1.4	
2	0.8	-0.6	-0.1	-1.3(±0.2)	

^a Incomplete (Ref. 10).

$E_{dd}=0$ in Eq. (6a) and it applies to both spin-dependent and spin-independent correlations. For spin-zero bosons this would be the only source of error in the HNC theory. We have repeated our calculation assuming Bose statistics for $\rho = 0.016 \text{ \AA}^{-3}$ and find an energy of -2.4 K . The Monte Carlo evaluation of this energy¹² gives -2.9 K and the error in the HNC approximation is about 0.5 K . This error will be significantly smaller for fermions, however, because the elementary diagrams contributing to E_{dd} all have at least two internal points which may be either exchanged with one another or not. There will be a substantial cancellation between these two possibilities (which should be almost complete for the polarized system).

The second source of error applies only to spin-dependent correlations where we have calculated correctly only diagrams with a ladder structure or those with single rings of spin correlations. The leading correction to this approximation is through vertex corrections to the effective interaction of Eq. (4b) (Refs. 5 and 6). We have calculated the leading vertex correction and find that it raises the energy by about 0.01 K . This is less than 4% of the energy lowering due to the spin correlations.

Finally, let us remark on the choice (2) of spin-correlation function. In second-order perturbation theory⁴ the correlation function between particles in momentum states \vec{k}_i and \vec{k}_j , which scatter by transferring momentum \vec{k} , is independent of their spin states and has the following form:

$$u(i,j) = u(k) [\vec{k} \cdot (\vec{k} - \vec{k}_i + \vec{k}_j)]^{-1}. \quad (8)$$

The correlation function (2) is an approximation to this state dependence which distinguishes only whether the particles occupy even or odd relative partial waves by distinguishing whether they occupy a singlet or a triplet spin state. The averaging over \vec{k}_i and \vec{k}_j , which gives a correlation function of the form (2), loses the pole at $\vec{k} = \vec{k}_i - \vec{k}_j$ in expression (8). This pole should determine the long-range r -space or small- k behavior of the contribution to the distribution function which comes from the scattering of a pair of particles in exchange states. Although

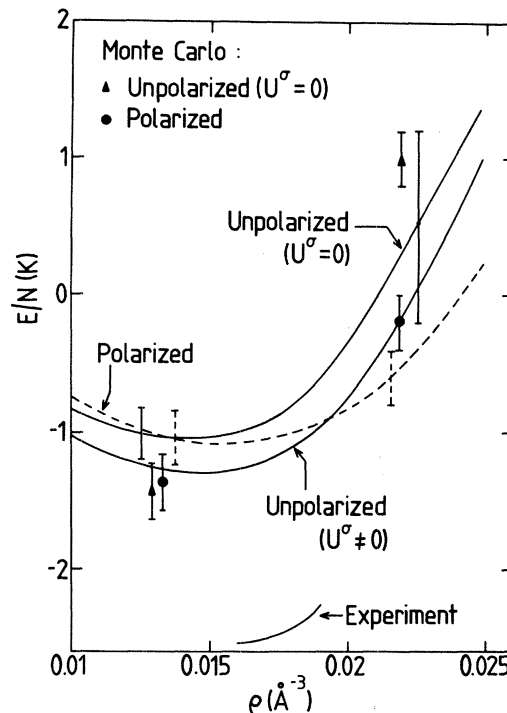


FIG. 2. The energy per particle in the polarized and unpolarized phases with spin-independent ($u^\sigma = 0$) and spin-dependent ($u^\sigma \neq 0$) correlations. All calculations used the Lennard-Jones potential.

the correlation function (2) may be reasonable for evaluating the energy, it does not give a proper description of the long-range structure of the wave function in exchange states. This means, for example, that our calculation does not give a good description of the spin-dependent structure function in the small- k limit, nor can we establish a connection between the existence of solutions to the Euler equations and local stability.

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¹D. Levesque, Phys. Rev. B **21**, 5159 (1981); C. Lhuillier and D. Levesque, *ibid.* **23**, 2203 (1981).

²G. S. Rushbrooke, G. A. Baker, and P. J. Wood, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1974), Vol. 3.

³G. Ripka, Nucl. Phys. **A314**, 115 (1979); J. C. Owen and G. Ripka, Lectures at Summer School for Nuclear Physics, University of California, Santa Barbara, 1981 (Springer-Verlag, New York, in press).

⁴J. C. Owen, Phys. Lett. **82B**, 23 (1979).

⁵V. R. Pandharipande and R. B. Wiringa, Rev. Mod. Phys. **51**, 821 (1979).

⁶J. C. Owen, Ann. Phys. (N.Y.) **118**, 373 (1979).

⁷J. C. Owen, Phys. Rev. B **23**, 2169 (1981).

⁸E. Krotscheck, Phys. Rev. A **15**, 397 (1977).

⁹F. Y. Wu and E. Feenberg, Phys. Rev. **128**, 943 (1962).

¹⁰The inclusion of all third-order direct diagrams reduces this contribution by about 30%. The evaluation of all third-order exchange diagrams would present severe numerical problems.

¹¹E. K. Kurten and C. E. Campbell, J. Low Temp. Phys. **44**, 149 (1981); E. Krotscheck, R. A. Smith, J. W. Clark, and R. M. Panoff, Phys. Rev. B **24**, 6383 (1981).

¹²K. E. Schmidt *et al.*, Phys. Rev. Lett. **47**, 807 (1981).