

K. E. Kürten and C. E. Campbell

School of Physics and Astronomy
University of Minnesota
Minneapolis, Minnesota 55455, U.S.A.

ABSTRACT

Including a dependence on the z-component of the nuclear spin in the Jastrow wave function gives a substantial contribution to the ground state energy of liquid ${}^3\text{He}$, which tends to stabilize unpolarized liquid ${}^3\text{He}$ relative to completely polarized ${}^3\text{He}$.

INTRODUCTION

Variational calculations of the zero temperature equation of state of liquid ${}^3\text{He}$ including the dependence upon magnetization have given the result that the stable phase has a non-zero magnetization [1-3], in contradiction to the experimental situation. The trial wave function used in these calculations is a state independent Jastrow function

$$\Psi(r_1 \dots r_N, M) = \Psi_c(r_1 \dots r_N) \Phi_M(r_1 \sigma_1 \dots r_N \sigma_N) \quad (1)$$

where the correlation factor Ψ_c has the Jastrow form

$$\Psi_c(r_1 \dots r_N) = \prod_{i,j}^N f(r_{ij}) \quad (2)$$

and Φ_M is the ground state Slater determinant with total magnetization M. Since one of the variational calculations is a Monte Carlo evaluation of the expectation value of the Hamiltonian with respect to Ψ [3], thereby avoiding the uncertainties due to integral equation approximations such as used in the other calculations [1,2,4], the conclusion is that the class of trial functions defined by Eqs. (1) and (2) is not large enough to represent properly the sensitivity of the energy to M.

Several elaborations of the class of trial functions have been considered for unpolarized ${}^3\text{He}$, including using a sum of Slater determinants for Φ [5], including three-body factors in Ψ_c [6], and a combination of those two, [7]. While each of these will give energy shifts which depend upon M and therefore may put the

*Work supported in part by NSF grant DMR-7926447 and by the Deutsche Forschungsgemeinschaft. (Ku 446/1,2).

final result into better agreement with experiment, it is also plausible that including spin dependent correlation in Ψ_C will account for much of the relative shifts in the energy due to the magnetization. Indeed, spin dependent correlations will have little or no effect on the completely saturated state where the z components of the spins are all aligned, and should have maximum effect on the unpolarized phase where on average half of the z components are up and half down. Moreover, since we are enlarging the class of trial functions, the energy of the unpolarized state will be lowered relative to the polarized state. The quantitative question is whether the shift in energy is enough to overcome the energy difference.

σ_z - DEPENDENT THEORY

In an attempt to assess the size of such an effect, we have considered a trial function of the form of Eq. (1) but with the Jastrow factor depending on the z component of the nuclear spins, σ_i :

$$\Psi_C = \prod_{i < j} f(r_{ij}, \sigma_i, \sigma_j) \quad (3)$$

where

$$f(r_{ij}, \sigma_i, \sigma_j) = \exp \frac{1}{2} \left[\frac{1 + \sigma_i \sigma_j}{2} u_p(r_{ij}) + \frac{1 - \sigma_i \sigma_j}{2} u_d(r_{ij}) \right]. \quad (4)$$

This has the advantage that the commutators of the components of the spin $\vec{\sigma}_i$ do not enter the calculation [8]. Moreover, the trial function for the completely polarized state is unchanged from the σ_z independent case, since $\sigma_i = 1$ for all i. Consequently the energy of the unpolarized state will be lowered (algebraically), possibly becoming the preferred phase in agreement with experiment.

To calculate the energy expectation value we need certain two and three body distribution functions for the trial wave function [9]. The two-body functions arise naturally in the Fermi-hypernetted chain (FHNC) resummation of the cluster expansion for the radial distribution function [9,10]. To generalize to the σ_z dependent case, we note that the FHNC resummation is not changed in any essential way when discrete degrees of freedom are included in the wave function as discrete variables, as long as the distribution functions are expressed in terms of the variables $x_i = (r_i, \sigma_i)$.

The spin dependent radial distribution function is defined by

$$g(x_i, x_j) = (\nu/\rho)^2 N(N-1) \int |\Psi(x_i, \dots, x_N)|^2 dx_j \dots dx_N / \langle \Psi | \Psi \rangle$$

where the integral over x_i includes the sum over the z components of the spins and ν is the degeneracy due to the discrete variable. The FHNC expression for g can be motivated by noting that the wave function squared can be written as the product of the Jastrow function squared multiplied by the determinant of the square of the Slater matrix:

$$|\Psi(x_1, \dots, x_N)|^2 = \left[\prod_{i < j} f^2(x_i, x_j) \right] \text{Det } \beta(x_i, x_j) \quad (5)$$

where $\beta(x_i, x_j) = \beta(k_f r_{ij}) \delta_{\sigma_i \sigma_j} / 2$ and $\beta(z)$ is the Slater function $\beta(z) = 3(\sin z - z \cos z) / z^3$. The (boson) hypernetted chain resummation (HNC) applies for a function of the form of Eq. (5) but with $\text{Det } \beta_{ij}$ replaced by 1 [11]. The determinant factor in the fermion case introduces directed exchange bonds $\beta(x_i, x_j)$ which must be chained to form permutation polygons. Fantoni and Rosati [10] and Krotscheck and Ristig [12] showed how to incorporate these new bonds into the HNC resummation to produce the FHNC method.

It is convenient to decompose the $g(x_1, x_2)$ into several parts according to the exchange character of the external points 1 and 2 [13].

$$g(x_1, x_2) = g_{dd}(x_1, x_2) + 2g_{de}(x_1, x_2) + g_{ee}(x_1, x_2) \quad (6)$$

where e means that the external point is connected by an exchange bond to some other point and d means that it is not. It is necessary for later purposes to single out part of g_{ee} which has an exchange connection directly between points 1 and 2:

$$g_{ee}(x_1, x_2) = \Gamma_{ee}(x_1, x_2) - 2\beta(x_1, x_2) g_{ee}(x_1, x_2) \quad (7)$$

Then the principal features of the Fantoni-Rosati form of the FHNC equations are made explicit in terms of the direct correlation functions, X_{dd} , X_{de} , X_{cc} , and X_{ee} (also known as the non-nodal functions) associated with these four components of the radial distribution function, which are defined by

$$\Gamma_{dd}(x_{12}) = X_{dd}(x_{12}) + \frac{2}{V} \int dx_3 \{ X_{dd}(x_{13}) g_{de}(x_{32}) + [X_{dd}(x_{13}) + X_{de}(x_{13})] \Gamma_{dd}(x_{32}) \} \quad (8)$$

$$\equiv X_{dd}(x_{12}) + N_{dd}(x_{12})$$

$$g_{ee}(x_{12}) = \beta(k_f r_{12}) \delta_{\sigma_1 \sigma_2} + X_{ee}(x_{12}) - \frac{2}{V} \int dx_3 X_{ee}(x_{13}) g_{ee}(x_{32}) \quad (9)$$

$$\equiv \beta(k_f r_{12}) \delta_{\sigma_1 \sigma_2} + X_{ee}(x_{12}) + N_{ee}(x_{12})$$

$$g_{de}(x_{12}) = X_{de}(x_{12}) + \frac{2}{V} \int dx_3 \{ X_{dd}(x_{13}) g_{ee}(x_{32}) + [X_{dd}(x_{13}) + X_{de}(x_{13})] g_{de}(x_{32}) \} \quad (10)$$

$$\equiv X_{de}(x_{12}) + N_{de}(x_{12})$$

$$g_{ee}(x_{12}) = X_{ee}(x_{12}) + \frac{2}{V} \int dx_3 \{ X_{ed}(x_{13}) g_{ee}(x_{32}) + [X_{ed}(x_{13}) + X_{ee}(x_{13})] g_{de}(x_{32}) \} \quad (11)$$

where $\Gamma_{dd} = g_{dd} - 1$, and $N_{\alpha\beta}$ are the nodal functions.

The relationship between the $g_{\alpha\beta}$ (or $X_{\alpha\beta}$) and the correlation function $f^{\dagger}(x_1, x_2)$ is given by the hypernet equations, which are obtained by summing all parallel connections of the chains:

$$g_{dd}(x_{12}) = f^{\dagger}(x_1, x_2) \exp [N_{dd}(x_{12}) + E_{dd}(x_{12})] \quad (12)$$

$$g_{ee}(x_{12}) = g_{dd}(x_{12}) [\beta(k_f r_{12}) \delta_{\sigma_1 \sigma_2} + N_{ee}(x_{12}) + E_{ee}(x_{12})] \quad (13)$$

$$g_{de}(x_{12}) = g_{dd}(x_{12}) [N_{de}(x_{12}) + E_{de}(x_{12})] \quad (14)$$

$$g_{ee}(x_{12}) = g_{dd}(x_{12}) \left\{ N_{ee}(x_{12}) + E_{ee}(x_{12}) - [\beta(k_f r_{12}) \delta_{\sigma_1 \sigma_2} + N_{ee}(x_{12}) + E_{ee}(x_{12})]^2 + [N_{de}(x_{12}) + E_{de}(x_{12})]^2 \right\} - N_{ee}(x_{12}) \quad (15)$$

While these equations are exact, they contain the new functions $E_{\alpha\beta}(x_{12})$ which can only be defined as the sum of an infinite set of elementary diagrams, which are those diagrams which are non-nodal and not parallel connected at points 1 and 2.

The simplest approximation known as FHNC/0 is to set all $E_{\alpha\beta} = 0$. This is the natural fermion generalization of the HNC approximation, Zabolitzky has solved the FHNC/4 approximation, which includes dressed four-body elementary diagrams [14]. Comparison to Monte Carlo simulations [15] indicates that this approximation scheme is converging. Krotscheck and Ristig devised a different scheme for approximating these equations, resulting in improved long wavelength behavior of the structure factors [12]. The results for the polarized and unpolarized ${}^3\text{He}$ obtained by Clark et al. [2] use still another approximation scheme, FHNC/C [16], which preserves the long-range properties by an analytic estimate of the elementary diagrams omitted in the FHNC/0 approximation.

In liquid ${}^3\text{He}$ the discrete variable is the projection of the nuclear spin along some axis. Then $\nu = 2$, and the two values are labeled by $\sigma_i = \pm 1$ ("up" and "down"). Thus the hypernet equations and the chain equations each contain 16 coupled members, although that number is immediately halved by the symmetry between up and down. However, by choosing an appropriate representation for the spin dependence, the hypernet equations and the chain equations each become two sets of four equations not coupled one to the other which are nearly identical to the familiar spin summed FHNC equations.

Since the trial function $f(x_i, x_j)$ depends only on the interparticle distance r_{ij} and the correlations between the spins σ_i and σ_j , it can be written in the form

$$f(x_i, x_j) = f^{(0)}(r_{ij}) + \sigma_i \sigma_j f^{(\sigma)}(r_{ij}) \quad (16)$$

Moreover, since $\sigma_i^2 = 1$, all of the other two body functions ($g, \beta, g_{\alpha\beta}, X_{\alpha\beta}, N_{\alpha\beta}$) have the same form [17],

$$A(x_i, x_j) = A^0(r_{ij}) + \sigma_i \sigma_j A^\sigma(r_{ij}) \quad (17)$$

An alternative representation of the spin dependence of all of these functions is in terms of their spin parallel and spin anti-parallel part:

$$A(x_i, x_j) = \frac{1 + \sigma_i \sigma_j}{2} A^P(r_{ij}) + \frac{1 - \sigma_i \sigma_j}{2} A^A(r_{ij}) \quad (18)$$

The new two-body functions in (17) and (18) have the trivial relationship

$$A^0 = \frac{1}{2}(A^P + A^A) \quad , \quad A^\sigma = \frac{1}{2}(A^P - A^A) \quad (19)$$

Note in particular that the radial distribution function, which is the spin average of $g(x_i, x_j)$ is the component $g^0(r_{ij})$ and similarly for the components g_{dd} , g_{de} , and g_{ee} . The exception is the g_{cc} where the fact that $\delta_{\sigma_i \sigma_i} = \frac{1}{2}[1 + \sigma_i \sigma_i]$ means that

$$g_{cc}(r_{12}) = g_{cc}^\sigma(r_{12}) = \frac{1}{2} g_{cc}(r_{12}) \quad (20)$$

with a similar relation for X_{cc} and N_{cc} , where $g_{cc}(r_{12})$ is the usual cc function of the spin independent theory.

The convolution form of the chain equations (Eq. 8-11) and the fact that

$$\frac{1}{\nu} \sum_{\sigma_3} A(x_1, x_3) B(x_3, x_2) = A^0(r_{13}) B^0(r_{32}) + \sigma_1 \sigma_2 A^\sigma(r_{13}) B^\sigma(r_{32}) \quad (21)$$

can be used to show that the chain equations for the A^σ type functions separate from the A^0 type. Thus equations (8-11) become two sets of equations, one

containing only the superscript (σ) functions, the other set only the superscript (0), the only other change being that $\frac{1}{2} \int dx_3(\cdot)$ is replaced by $\int dx_3(\cdot)$. For example, the dd equation (Eq. (8)) is replaced by

$$\Gamma_{dd}^{\mu}(r_{12}) = \Sigma_{dd}^{\mu}(r_{12}) + \rho \int dx_3 \left\{ \Sigma_{dd}^{\mu}(r_{13}) g_{de}^{\mu}(r_{32}) + [\Sigma_{dd}^{\mu}(r_{13}) + \Sigma_{de}^{\mu}(r_{13})] \Gamma_{dd}^{\mu}(r_{32}) \right\} \quad (22)$$

where $\mu = 0$ or σ . In the cc equation, Eq. (9), $l(k_f r_{12}) \delta_{\sigma_1 \sigma_2}$ is to be replaced by $\frac{1}{2} l(k_f r_{12})$ or equivalently, using equation (20), Eq. (9) is replaced by

$$g_{cc}(r_{12}) = l(k_f r_{12}) + \Sigma_{cc}^{\mu}(r_{12}) - \frac{\rho}{2} \int dx_3 \Sigma_{cc}^{\mu}(r_{13}) g_{cc}^{\mu}(r_{32}), \quad (23)$$

which is independent of (μ) and is not coupled directly to any of the other three chain equations.

Note also that the hypernet equations (12-15) decouple in the spin parallel and anti-parallel projections defined in Eq. (18), since these equations depend explicitly on only the two external points 1 and 2. It is only necessary to put a superscript (p) or (a) on each function in Eq. (12-15) to obtain the spin parallel (or antiparallel) equations, and replace all of the arguments (x_1, x_2) by r_{12} . Note that the anti-parallel part of g_{cc} (i.e. g_{cc}^a) vanishes; consequently the first quadratic term inside the braces in the ee anti-parallel version of Eq. (15) vanishes.

RESULTS AND DISCUSSION.

Since our objective is an estimate of the sensitivity of the trial ground state of liquid ^3He to spin dependent correlations, it should be sufficient to use the simplest approximation, FHNC/0, and the commonly used Lennard-Jones 6-12 potential for the He-He interaction: $v(r) = 4\epsilon [(\sigma/r)^{12} - (\sigma/r)^6]$ with $\epsilon = 10.22$ K and $\sigma = 2.556$ A. We use the McMillan-Schiff-Verlet form for the Jastrow pseudo-potentials [18]

$$u_{\alpha}(r) = (b_{\alpha}/r)^{n_{\alpha}}, \quad \alpha = p \text{ or } a, \quad (24)$$

where b_p , n_p , b_a , and n_a are variational parameters. The spin-independent trial function corresponds to the choice $u_p = u_a$. The variational parameters are chosen independently for the three cases: unpolarized spin independent, unpolarized spin dependent, and completely polarized. We calculated the energy using the Jackson-Feenberg (JF) form of the kinetic energy [9] which we regard as most reliable for a variational calculation since it depends only very weakly on the three-body distribution function (which must have a further approximation such as the superposition approximations). Within the numerical accuracy of our calculation, the parameter $n_p = n_a = 5$, and the range parameters b_p and b_a are nearly independent of density to within ± 0.01 Å (except at the lowest density).

The energy per particle is given in Figure 1 for unpolarized liquid ${}^3\text{He}$ with no state dependence in the Jastrow function ($u_p = u_a$) and with σ_z dependent Jastrow function. In the σ_z independent case $b_p = b_a = 2.89 \text{ \AA}$ for $\rho \geq 0.0142 \text{ \AA}^{-3}$, while in the σ_z dependent case $b_p = 2.94 \text{ \AA}$ and $b_a = 2.83 \text{ \AA}$. The numerical uncertainty of the energies is $\pm 0.03 \text{ K}$, but increases somewhat near the highest densities plotted (there is a systematic error in this approximation which increases with density but cannot be estimated until more sophisticated approximations (such as /4) are tried). At experimental equilibrium density 0.0164 \AA^{-3} the contribution of the σ_z correlations to the energy is -0.27 K per particle, and it grows with density. Thus the calculated equilibrium density is increased somewhat.

Also shown in Fig. 1 is the energy per particle for polarized ${}^3\text{He}$ calculated in the FHNC/O approximation. The variational parameter b is 2.80 \AA in this case. The smaller value than the unpolarized case is as would be expected from the fact that the Pauli exclusion principle is of more aid in reducing the repulsive energy in the polarized case than in the unpolarized case. Note, however, that $b_p > b_a$ in the unpolarized σ_z dependent case, contrary to expectations. This suggests that the attractive part of the potential energy plays an important role in the difference between u_p and u_a . Significant conclusions about the σ_z effects on the structure of the wave function should, however, await solutions to the Euler-Lagrange equations for u_p and u_a ; the present parameter variations are to be trusted only for the energy differences.

In Figure 2, our results for the difference between the polarized energy and the state independent unpolarized energy are shown to lie within the error bars of Levesque's results [3]. Included for comparison are recent results of Krotscheck et al. [2] using a state independent Euler-Lagrange calculation in the /C approximation which are seen to fall below the other results and thus even favor the polarized phase more.

In summary, we have shown that σ_z dependent contributions to the ground state energy of liquid ${}^3\text{He}$ are not insignificant. Moreover, the variational principle implies that the spin-dependent energy shift would be even larger if the Jastrow correlation factor depended on the full quantum mechanical spin in the form $\vec{\sigma}_i \cdot \vec{\sigma}_j$ which by symmetry arguments is preferable to $\sigma_{iz} \sigma_{jz}$. This introduces the complication of non-commuting f operators in the Jastrow function which makes it difficult to estimate the energy shift. It is a straightforward matter, however, to calculate the $\vec{\sigma}_i \cdot \vec{\sigma}_j$ contribution in second-order perturbation theory, where it is easy to see formally that the energy shift is tripled when going from a $\sigma_{iz} \sigma_{jz}$ dependence to $\vec{\sigma}_i \cdot \vec{\sigma}_j$ dependence [19]. It can be seen from the results in Fig. 2 that three times the σ_z shift would be a very important contribution to stabilizing the unpolarized phase relative to the polarized phase. While the factor of three may be too large (there are no commutator effects), these results suggest that a

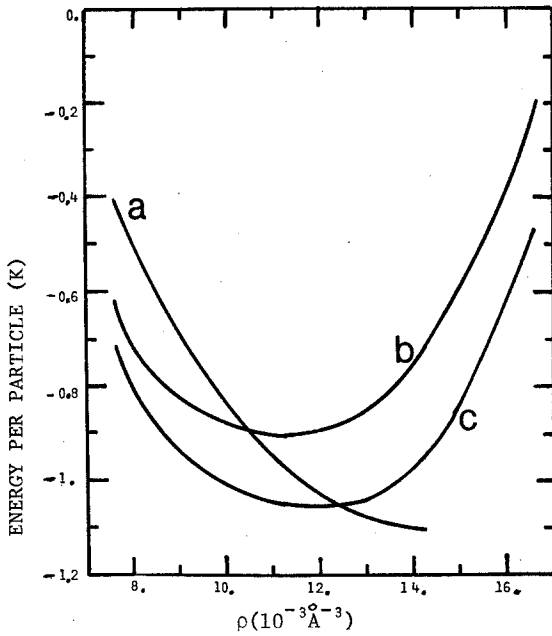


Fig. 1. Jastrow ground-state energy versus density for A, polarized ^3He ; B, unpolarized ^3He state independent; C, unpolarized ^3He state dependent.

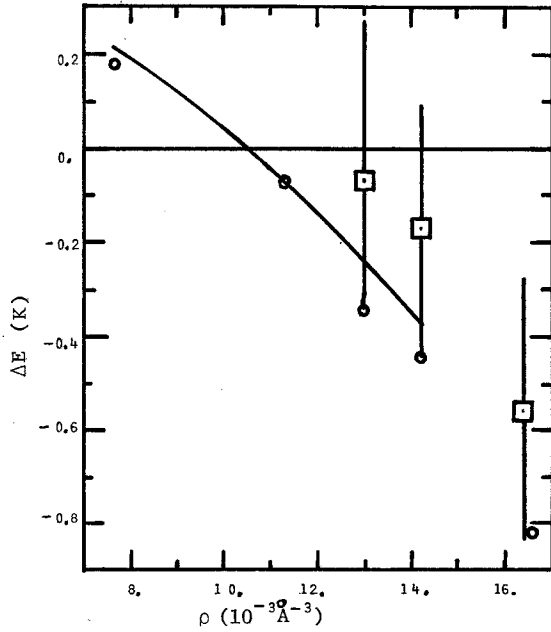


Fig. 2. Energy differences between the polarized energy and the state independent unpolarized energy versus density. \square , Levesque [3]; \circ Clark et al. [2]; solid line, present calculation.

full spin-dependent Jastrow calculation for liquid ^3He should have a high priority.

We would like to acknowledge helpful discussions with M. Ristig.

REFERENCES

1. R. A. Guyer and M. D. Miller, Phys. Rev. B18, 3521 (1978); Phys. Rev. B21, 3917 (1980).
2. J. W. Clark, E. Krotscheck and R. M. Panoff, J. Phys. Colloq. (Paris), to be published; E. Krotscheck, R. A. Smith, J. W. Clark and R. M. Panoff, to be published.
3. D. Levesque, Phys. Rev. B12, 5159 (1980).
4. M. L. Ristig, P. M. Lam and H. P. Nollert, J. Phys. Colloq. (Paris) to be published.
5. C. W. Woo, Phys. Rev. 151, 138 (1966); H. T. Tan and E. Feenberg, Phys. Rev. 176, 360 (1968).
6. C. E. Campbell, Phys. Lett. 44A, 471 (1973); C. Chang and C. E. Campbell, Phys. Rev. B15, 4238 (1977); V. R. Pandharipande, Phys. Rev. B18, 218 (1978).
7. K. Schmidt and V. R. Pandharipande, Phys. Rev. B19, 2504 (1979).
8. R. A. Smith, Nucl. Phys. A328, 169 (1979).
9. J. W. Clark, Progress in Particle and Nuclear Physics, Vol. 2, pg. 89 (ed. by D. H. Wilkinson, Pergamon, Oxford, 1979).
10. S. Fantoni and S. Rosati, Nuovo Cim. 25A, 593 (1975).
11. J. M. J. van Leeuwen, J. Groeneveld, and J. deBoer, Physica 25, 792 (1959); T. Morita, Prog. Theor. Phys. 23, 829 (1960).
12. E. Krotscheck and M. L. Ristig, Nucl. Phys. A242, 389 (1975).
13. E. Krotscheck, Z. Physik B32, 395 (1979).
14. J. G. Zabolitzky, Phys. Rev. A16, 1258 (1977).
15. M. H. Kalos, Nucl. Phys. A328, 153 (1979), and ref. cited therein.
16. E. Krotscheck, Nucl. Phys. A317, 149 (1979).
17. M. L. Ristig, K. E. Kürten and J. W. Clark, Phys. Rev. B19, 3539 (1979).
18. W. L. McMillan, Phys. Rev. 138, A442 (1965); D. Schiff and L. Verlet, Phys. Rev. 160, 208 (1967).
19. C. E. Campbell, K. E. Kürten and E. Krotscheck, work in progress.