

Energy and structure of the ground state of liquid ${}^4\text{He}^\dagger$

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We present the results of a calculation of the energy- and liquid-structure function of the ground state of liquid ${}^4\text{He}$ in the density range $0.0180\text{--}0.0257 \text{ \AA}^{-3}$, using both the Lennard-Jones 6-12 potential and the second Morse-dipole-dipole potential of Bruch and McGee. The method is to determine the optimum Jastrow trial wave function by multiple iteration of the paired-phonon analysis, and then calculate the contributions of three-body factors in the wave function. Tables of values are given at several densities for the radial distribution function, Jastrow function, and liquid-structure function. We also present a variational formulation of the paired phonon analysis and numerical examples of its convergence and self-consistency.

I. INTRODUCTION

In this paper we present the results of a calculation of the energy and structure of the ground state of liquid ${}^4\text{He}$. Our method of calculation is to solve the equations generated by functional variations of the expectation value of the Hamiltonian in Jastrow and extended Jastrow functions. Results are presented for the density range $\rho = 0.0180\text{--}0.0257 \text{ \AA}^{-3}$, which includes the experimentally observed density range of the liquid. Two commonly used phenomenological interaction potentials are used, enabling us to investigate the sensitivity of the results to the potential.

We begin with a brief introduction to the variational theory of the ground state of liquid ${}^4\text{He}$. Sections II and III contain a discussion of the paired-phonon analysis, which is the method used for solving the Jastrow variational problem. The results of the Jastrow calculation are given in Sec. IV, followed by an estimation of three-body extended Jastrow corrections in Sec. V. The reader interested only in the results of our calculation and not in the supporting formalism may omit Secs. II and III.

The theory of the ground state of liquid ${}^4\text{He}$ has been the subject of much work during the last decade.¹⁻³ The principal experimental information about the ground state is the ground-state energy E_0 and liquid-structure function $S(k)$. Both are measured at low temperatures and then extrapolated to zero temperature to give the corresponding ground-state values, defined by

$$H\Psi_0 = E\Psi_0 \quad (1)$$

and

$$S(k) = (1/N)\langle\Psi_0|\rho_{\vec{k}}\rho_{-\vec{k}}|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle, \quad (2)$$

where Ψ_0 is the ground-state wave function, H is the Hamiltonian for the N helium atoms, and $\rho_{\vec{k}}$ is the density fluctuation operator

$$\rho_{\vec{k}} = \sum_{i=1}^N e^{i\vec{k}\cdot\vec{r}_i}. \quad (3)$$

A straightforward approach to the theory of the ground state which has given reasonably good agreement with these experimental quantities is the Jastrow variational theory, where the ground-state wave function Ψ_0 is approximated by a trial function of the Jastrow form Ψ_J :

$$\Psi_J(\vec{r}_1, \dots, \vec{r}_N) = \prod_{i<j}^N e^{u(r_{ij})/2}. \quad (4)$$

The variational principle tells us that the expectation value of the Hamiltonian in Ψ_J provides an upper bound on the ground-state energy

$$E_J \equiv \langle\Psi_J|H|\Psi_J\rangle/\langle\Psi_J|\Psi_J\rangle \geq E_0. \quad (5)$$

Variational calculations to optimize this upper bound are usually carried out by considering a $u(r)$ with a few parameters, most frequently⁴⁻⁶

$$u(r) = -(b/r)^p, \quad (6)$$

and then minimizing E_J with respect to these parameters (b and p in this case). Except for the long-wavelength structure⁷ this simple form has produced reasonably good agreement with experiment.

The several methods for calculating the expectation value E_J fall into two categories: essentially exact calculations for $10^2\text{--}10^3$ particles; and approximate integral equations for infinite systems. The first of these simply uses the Monte Carlo^{4,6} or molecular-dynamics⁵ integration of the expectation value for the finite system. Most of these calculations have used the Lennard-Jones 6-12 potential with the deBoer-Michels parameters [Eq. (63) below], obtaining $p=5$ and $b=3.0 \text{ \AA}$ at the experimental equilibrium density ($\rho_0 = 0.02185 \text{ \AA}^{-3}$). Murphy has investigated several potentials, using

the variational principle to set limits on the parameters of these potentials so that E_J does not fall below the experimental energy at any measured density.⁸

The uncertainties in these Monte Carlo and molecular-dynamics calculations are due to finite size of the system and to the fact that only a finite number of configurations can be sampled. These errors can be eliminated, for a price, by introducing approximations such as the hypernetted-chain approximation⁸ (HNC), the Percus-Yevick approximation⁸ (PY), or the Kirkwood superposition truncation of the Bogoliubov-Born-Green-Kirkwood-Yvon⁹ (BBGKY) hierarchy (BBGKY-KSA). The price is that these approximations produce systematic errors. These errors may be estimated by some reference procedure. We discuss one such procedure below.

While these parameter variations have led to a reasonably good accounting of the experimental energy and structure near the equilibrium density for liquid ⁴He, improvements can be expected if a wider space of variational functions can be easily sampled. For example, it is expected that the best $u(r)$ has a more complicated structure than the simple monotonic form of Eq. (6), particularly at long wavelengths and at high densities. Furthermore, this short-range structure of $u(r)$ is adequate only for the 6-12 potential (and then $p = 5$).

Several years ago, Feenberg and one of us (C.E.C.) showed how to obtain the optimum Jastrow function (in the variational sense) from the class of all Jastrow functions.¹⁰ It was shown that a partial diagonalization of the Hamiltonian introduced earlier by Jackson and Feenberg as a theory of the quasiparticle model¹¹ (referred to as the paired-phonon analysis) has as its ground state the optimum Jastrow wave function. In Sec. II we give an alternative (and we believe simpler) derivation of this result for the ground state by a direct application of the variational principle.

From an operational point of view, the application of the paired-phonon analysis to the problem of determining the optimum Jastrow trial function requires two choices. Both of these choices are discussed in Sec. III. The first is the choice of which procedure to use for calculating the energy from a given Jastrow function, be it an "exact" procedure such as Monte Carlo integration, or an approximation such as PY or HNC. We discuss the self-consistency condition for choosing amongst the various approximations which are available or may become available.¹² The second choice comes about because the paired-phonon analysis is a predictor-corrector scheme when applied to the ground-state problem, and, as such requires an initial choice of Jastrow trial function. The paired-

phonon analysis produces a new Jastrow trial function which is an improvement over the initial choice in the sense that the expectation value of the Hamiltonian is lowered. The new Jastrow function is then used as the initial Jastrow function for a repetition of this procedure, which is then iterated until successive iterations produce negligible change. The final Jastrow function is the variational optimum Jastrow function from amongst all possible Jastrow functions, independent of any particular choice of parametrization.¹⁰ In particular, it should not depend upon the original Jastrow function in this iterative procedure. In Sec. III we demonstrate by example the insensitivity of the optimum Jastrow function to the beginning function of the iteration. On the other hand we note that the rate of convergence to the optimum function is sensitive to the initial choice.

In this paper we restrict our calculations to the HNC approximation since it is the simplest self-consistent approximation in the sense discussed in Sec. III. In Sec. IV we use a reference procedure for correcting the errors due to this approximation. We calculate our estimates for the ground-state energy and liquid-structure function at several densities and for two choices of the He-He interaction: the Lennard-Jones 6-12 potential and the second Morse-dipole-dipole (MDD-2) potential.

While the results of Sec. IV give reasonable results for some of the properties of liquid ⁴He, recent interest has been focussed on enlarging the class of trial functions beyond the Jastrow form [Eq. (4)] to obtain further improved agreement with experiment.¹³⁻¹⁵ This is accomplished by noting that the Bose ground-state wave function can be chosen as real and positive semidefinite, and thus may be written in the form^{14,13}

$$\Psi_0(\vec{r}_1, \dots, \vec{r}_N) = \exp[\frac{1}{2}\phi(\vec{r}_1, \dots, \vec{r}_N)], \quad (7)$$

where ϕ may be resolved into a sum of n -body short-range functions

$$\phi(\vec{r}_1, \dots, \vec{r}_N) = \sum_{n=1}^N \frac{1}{n!} \sum_{\substack{i_1, \dots, i_n \\ i_p \neq i_q}} u_n(\vec{r}_{i_1}, \dots, \vec{r}_{i_n}). \quad (8)$$

This form suggests a systematic approximation scheme whereby only a few terms in the sum over n are retained. For example, the Hartree approximation for a boson system is obtained by retaining only the $u_1(\vec{r})$ term in ϕ and determining it variationally. The Jastrow form is obtained by retaining $u_1(\vec{r})$ and $u_2(\vec{r}, \vec{r}')$ [$u_1(\vec{r}) = 0$ in a translational invariant system, and $u_2(\vec{r}, \vec{r}') = u(|\vec{r} - \vec{r}'|)$] to produce the form of Eq. (4)].

A parametrized variational calculation including three-body factors [u_3 in Eq. (8)] has been done by

Woo and Coldwell by using Monte Carlo integration for two-dimensional liquid ^4He .¹⁶ One of us has developed an optimization procedure for determining the best u_n ($n > 2$) similar to the paired-phonon analysis.¹⁴ We briefly review this formalism in Sec. V and give the results for the $n=3$ modifications to the energy- and liquid-structure functions at the same densities and potentials as in Sec. IV.

II. VARIATIONAL OPTIMIZATION OF THE JASTROW FUNCTION

In this section we derive a procedure for calculating the optimum Jastrow factor in a trial ground-state wave function for the boson system. The results of this section are identical to those obtained in the paired-phonon analysis in Ref. 10. The method we employ to derive these results is variational rather than an approximate diagonalization of the Hamiltonian.

We begin with an initial trial function Ψ_0 :

$$\Psi_0(\vec{r}_1, \dots, \vec{r}_N) = e^{\phi_0(\vec{r}_1, \dots, \vec{r}_N)^{1/2}}, \quad (9)$$

where all we specify about ϕ_0 is that it is real and has a well-behaved expectation value for the Hamiltonian. ϕ_0 can be resolved into n -body short-range functions as Eq. (8). In particular we write

$$\phi_0(\vec{r}_1, \dots, \vec{r}_N) = \sum_{i < j}^N u_0(r_{ij}) + \tilde{\phi}_0(\vec{r}_1, \dots, \vec{r}_N), \quad (10)$$

where $\tilde{\phi}_0$ contains no two-body terms. We shall not have to be more specific about $\tilde{\phi}_0$ until later.

We now suppose that the expectation value of the Hamiltonian can be lowered by a different choice of two-body function than u_0 , so that we seek an improved trial state in the form

$$\Psi(\vec{r}_1, \dots, \vec{r}_N) = \Psi_0(\vec{r}_1, \dots, \vec{r}_N) \exp\left(\frac{1}{2} \sum_{i < j}^N \Delta u(r_{ij})\right). \quad (11)$$

A formal statement of the variational problem which we wish to solve is

$$[\delta/\delta\Delta u(r)] \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle = 0. \quad (12)$$

A simpler expression of this variational condition is obtained by introducing the Fourier transform of $\Delta u(r)$:

$$\Delta u(r) = \frac{1}{N} \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}. \quad (13)$$

Then the function which appears in the exponential

in Eq. (11) is

$$\sum_{i < j}^N \Delta u(r_{ij}) = \frac{1}{2} \sum_{\vec{k}} c_{\vec{k}} (\rho_{\vec{k}} \rho_{-\vec{k}} / N - 1), \quad (14)$$

and Ψ takes the form

$$\Psi = \Psi_0 \prod_{\vec{k}} e^{-c_{\vec{k}}/4} \prod_{\vec{k}} \exp\left[\frac{1}{4} (\rho_{\vec{k}} \rho_{-\vec{k}} / N) c_{\vec{k}}\right]. \quad (15)$$

Note that with this definition the variational equation, Eq. (12), becomes

$$\langle \Psi | (H - E) \rho_{\vec{k}} \rho_{-\vec{k}} | \Psi \rangle = 0, \quad (16)$$

where

$$E = \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle. \quad (17)$$

To calculate the energy it is convenient to follow Jackson and Feenberg by introducing an auxiliary function¹¹

$$\tilde{V}(\vec{r}_1, \dots, \vec{r}_N) = V(\vec{r}_1, \dots, \vec{r}_N) - \frac{\hbar^2}{8m} \sum_{i=1}^N \nabla_i^2 \ln \Psi^2, \quad (18)$$

where m is the mass of the atoms and V is the total potential [ordinarily

$$V = \sum_{i < j}^N V(r_{ij}),$$

the sum of two-body potentials, but the formal analysis permits a general form for V]. The advantage of this function is that the energy is given by the expectation value of the function \tilde{V} :

$$E = \langle \Psi | \tilde{V} | \Psi \rangle / \langle \Psi | \Psi \rangle. \quad (19)$$

We next use two wave functions which depend upon a variable α :

$$\Psi(\alpha) = \Psi e^{\alpha \tilde{V}/2}, \quad \Psi_0(\alpha) = \Psi_0 e^{\alpha \tilde{V}_0/2}, \quad (20)$$

where \tilde{V}_0 is defined in Eq. (18) with Ψ_0 replacing Ψ . Then the normalization integrals of these two functions in Eq. (20) serve as the generating functions for the respective energies:

$$E = \left. \frac{d}{d\alpha} \ln I(\alpha) \right|_{\alpha=0}, \quad E_0 = \left. \frac{d}{d\alpha} \ln I_0(\alpha) \right|_{\alpha=0}, \quad (21)$$

where

$$I(\alpha) = \langle \Psi(\alpha) | \Psi(\alpha) \rangle, \quad (22)$$

$$I_0(\alpha) = \langle \Psi_0(\alpha) | \Psi_0(\alpha) \rangle.$$

The normalization integral $I(\alpha)$ may be written in the form

$$I(\alpha) = I_0(\alpha) \left(\prod_{\vec{k}, k_x > 0} e^{-c_{\vec{k}}(\alpha)} \langle \Psi_0(\alpha) | \prod_{\vec{k}, k_x > 0} e^{c_{\vec{k}}(\alpha) \rho_{\vec{k}} \rho_{-\vec{k}} / N} | \Psi_0(\alpha) \rangle \right) [\langle \Psi_0(\alpha) | \Psi_0(\alpha) \rangle]^{-1}, \quad (23)$$

where we define

$$c_{\vec{k}}(\alpha) = (1 + \alpha \hbar^2 k^2 / 4m) c_{\vec{k}}^*, \quad (24)$$

and we use the fact that $c_{\vec{k}} = c_{-\vec{k}}^* = c_{\vec{k}}^*$ [$\Delta u(r)$ is real and has inversion symmetry] to restrict the product over \vec{k} to a half-space.

With this set of definitions, the remaining task is to evaluate the last factor in Eq. (23) as a function of $c_{\vec{k}}$. That factor has the general form

$$J(\{y_{\vec{k}}\}) = \langle \chi_0 | \prod_{\vec{k}, k_x > 0} e^{y_{\vec{k}} \rho_{\vec{k}} - \vec{k} / N} | \chi_0 \rangle, \quad (25)$$

where χ_0 is some normalized state and $\{y_{\vec{k}}\}$ is a set of dummy variables. The function has been shown numerous times in the literature to be approximately given by^{10,17}

$$J(\{y_{\vec{k}}\}) \approx \prod_{\vec{k}, k_x > 0} [1 - y_{\vec{k}} S_0(k)]^{-1}, \quad (26)$$

where $S_0(k)$ is the liquid-structure function for the state χ_0 . We don't rederive this approximation here, but simply note that it is the result one obtains by retaining only second-order cumulants of the density fluctuation operators in the cumulant expansion of Eq. (25).¹⁷ This is the only approximation we use in this section, and we discuss its consequences below.

Equation (21) is used with this approximation (26) for the last factor in Eq. (23) to obtain for the energy

$$E = E_0 + \sum_{\vec{k}, k_x > 0} E_{\vec{k}} = E_0 + \Delta E, \quad (27)$$

where

$$E_{\vec{k}} = -\frac{\hbar^2 k^2}{4m} c_{\vec{k}} + c_{\vec{k}} \frac{(\hbar^2 k^2 / 4m) S_0(k) + \mathcal{J}(k)}{1 - c_{\vec{k}} S_0(k)}, \quad (28)$$

where we have defined

$$\mathcal{J}(k) = \frac{\partial}{\partial \alpha} S_0(k, \alpha) \Big|_{\alpha=0}, \quad (29)$$

where¹⁸

$$S_0(k, \alpha) = \frac{1}{N} \frac{\langle \Psi_0(\alpha) | \rho_{\vec{k}} \rho_{-\vec{k}} | \Psi_0(\alpha) \rangle}{\langle \Psi_0(\alpha) | \Psi_0(\alpha) \rangle}. \quad (30)$$

Minimizing $E_{\vec{k}}$ with respect to $c_{\vec{k}}$ gives

$$c_{\vec{k}} = \{1 - [S_0(k) + 4m\mathcal{J}(k)/\hbar^2 k^2]^{1/2}\} / S_0(k), \quad (31)$$

which gives

$$E_{\vec{k}} = -[\hbar^2 k^2 / 4m S_0(k)] \times \{1 - [S_0(k) + 4m\mathcal{J}(k)/\hbar^2 k^2]^{1/2}\}^2. \quad (32)$$

The liquid structure function for the new wave function Ψ may be obtained from the generating function J by

$$S(k) = \frac{\partial \ln J(\{c_{\vec{k}}\})}{\partial c_{\vec{k}}}, \quad (33)$$

with $\chi_0 = \Psi_0$. With the approximation in Eq. (26) this becomes⁷

$$S(k) = S_0(k) / [1 - c_{\vec{k}} S_0(k)]. \quad (34)$$

This completes the formal derivation of the shift in the wave function which produces the optimum Jastrow factor for the evaluation of the energy. We are still faced with the task of calculating $\mathcal{J}(k)$ and with the estimation of the error introduced by the approximation in Eq. (26). The evaluation of $\mathcal{J}(k)$ is taken up in Sec. III.

Concerning the error introduced by approximation (26), we note that the result of the calculation is a new wave function of the form of Ψ_0 , but with the Jastrow part $u_0(r)$ replaced by $u_0(r) + \Delta u(r)$. Consequently the new energy E may be evaluated directly by the same procedure as that used for E_0 . Similarly, the new liquid-structure function may be evaluated directly for the new wave function and compared to the approximation in Eq. (34). Because of the approximation Ψ will not be precisely the optimum wave function and thus this directly calculated energy and structure function will not agree exactly with the values calculated in Eqs. (27) and (34). The entire procedure can be iterated by treating Ψ as the initial wave function and calculating a new shift in the energy and structure function. With an adequately chosen initial Ψ_0 , this procedure will converge to the trial function with the optimum Jastrow factor in several iterations.¹⁰ In Sec. III we demonstrate by example that the final result of this iterative procedure is independent of the initial function u_0 . But the rate of convergence is sensitive to the choice of u_0 , and a poor choice of u_0 may result in no convergence at all.

III. SELF-CONSISTENT APPLICATION OF THE PAIRED-PHONON ANALYSIS

In this section we complete the analysis of Sec. II by discussing procedures for calculating the function $\mathcal{J}(k)$ defined in Eq. (29) and study in detail the application of the paired-phonon analysis at the experimental equilibrium density of liquid ⁴He.

Using the definition of $\Psi_0(\alpha)$ in Eq. (20), $\mathcal{J}(k)$ may be rewritten

$$\mathcal{J}(k) = N^{-1} \langle \Psi_0 | \vec{V}[\rho_{\vec{k}} \rho_{-\vec{k}} - NS_0(k)] | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle. \quad (35)$$

From Eq. (31) we see that the condition that the initial wave function has the optimum Jastrow factor (so that $c_{\vec{k}}$ vanishes) is¹⁰

$$\mathcal{J}(k) = (\hbar^2 k^2 / 4m) [1 - S_0(k)]. \quad (36)$$

It can be verified that this is equivalent to the variational condition stated in Eq. (16) with Ψ replaced by Ψ_0 .¹⁰

In principle $\mathcal{H}(k)$ may be calculated by using the Monte Carlo or molecular-dynamics integration routines for a finite number of particles. For a practical calculation we now restrict our attention to the Jastrow function space by setting $\tilde{\phi}_0 = 0$ in Eq. (10). Even with this restriction \tilde{V}_0 is the sum of two-body functions

$$\tilde{V}_0(\vec{r}_1, \dots, \vec{r}_N) = \sum_{i < j}^N \left(V(r_{ij}) - \frac{\hbar^2}{4m} \nabla_{ij}^2 u_0(r_{ij}) \right), \quad (37)$$

and thus, since it is multiplied by $\rho_{\vec{r}} \rho_{-\vec{r}}$ in Eq. (35), the three- and four-particle distribution functions are needed to evaluate $\mathcal{H}(k)$. Another way of illustrating the difficulty is to note that $\mathcal{H}(k)$ is a fluctuation and thus requires a much more accurate Monte Carlo or molecular-dynamics evaluation than is necessary for E_0 and $S_0(k)$.

It was pointed out in Ref. 10 that an alternative procedure is to make use of the formal similarity between the square of the Jastrow function and the Boltzmann factor of a classical system to generate approximations for $\mathcal{H}(k)$. Specifically, the radial distribution $g_0(r)$ for Ψ_0 is defined by

$$g_0(r) = \frac{N(N-1)}{\rho^2 \langle \Psi_0 | \Psi_0 \rangle} \int \exp \sum_{i < j}^N u_0(r_{ij}) d\vec{r}_3, \dots, d\vec{r}_N, \quad (38)$$

where ρ is the number density of the system and the integrand is just the square of the Jastrow function Ψ_0 . Using Eq. (19) for the energy shows that it only depends on g_0 :

$$E_0 = \frac{1}{2} N \rho \int g_0(r) \tilde{V}_0(r) d\vec{r}, \quad (39)$$

where

$$\tilde{V}_0(r) = V(r) - (\hbar^2/4m) \nabla^2 u_0(r). \quad (40)$$

It has been noted that the form of Eq. (38) is such that $g_0(r)$ is also the radial distribution function evaluated in the canonical ensemble for a fictitious classical fluid with two-body potential $\phi_{cl}(r)$ at temperature T chosen so that⁵

$$\phi_{cl}(r)/k_B T = -u_0(r). \quad (41)$$

With this observation it has been possible to take advantage of the numerous approximate relations between $\phi_{cl}(r)$ and $g_0(r)$ derived in the theory of classical fluids. These approximations are characterized by the fact that they have a closed functional form¹⁹

$$g_0(r) = F[u_0, g_0; r], \quad (42)$$

which is to be solved for $g_0(r)$. Two frequently

used approximations are the HNC and PY approximations which are defined below in Eqs. (55)–(58).

Having introduced an approximate relationship between $u_0(r)$ and $g_0(r)$ of the form of Eq. (42), we must examine again the variational calculation. Our objective is now defined as minimizing the energy self-consistently within the chosen approximation. The energy is *defined* by Eq. (39) where g_0 satisfies Eq. (42). Then the Euler-Lagrange equation for the optimum $u(r)$ is

$$\delta E / \delta u(r) = 0, \quad (43)$$

which from Eq. (39) is²⁰

$$\frac{\hbar^2 \nabla^2 g_0(r)}{4m} = \int \tilde{V}(r') \frac{\delta g_0(r')}{\delta u(r)} d\vec{r}'. \quad (44)$$

The functional derivative on the right-hand side may be evaluated within the approximation by

$$\frac{\delta g_0(r)}{\delta u(r')} = \frac{\delta F[u, g; r]}{\delta u(r')}. \quad (45)$$

We now have the extremum condition within the approximation given by these last two equations on one hand, and the paired-phonon optimization condition Eq. (36) on the other. In the absence of any approximation we observed that these two conditions are equivalent, which is the essential feature which makes the paired-phonon analysis a useful predictor-corrector procedure for generating the optimum Jastrow function.¹⁰ To compare these two conditions *within an approximation* like Eq. (42), we note that the definition of $\mathcal{H}(k)$, Eq. (29), may be written

$$\mathcal{H}(k) = \rho \int e^{-i\vec{k} \cdot \vec{r}} \left. \frac{\partial g_0(r, \alpha)}{\partial \alpha} \right|_{\alpha=0} d\vec{r}, \quad (46)$$

where $g_0(r, \alpha)$ is defined as in Eq. (38) but with $u_0(r, \alpha)$ replacing $u_0(r)$, where

$$u_0(r, \alpha) = u_0(r) + \alpha \tilde{V}_0(r) \quad (47)$$

[i.e., Ψ_0 is replaced by $\Psi_0(\alpha)$]. Then the paired-phonon optimization condition [Eq. (36)] may be Fourier transformed to give

$$\left. \frac{\partial g_0(r, \alpha)}{\partial \alpha} \right|_{\alpha=0} = \frac{\hbar^2}{4m} \nabla^2 g_0(r). \quad (48)$$

To compare this to Eq. (44), we use the chain rule for the left-hand side of (48):

$$\left. \frac{\partial g_0(r, \alpha)}{\partial \alpha} \right|_{\alpha=0} = \int d\vec{r}' \tilde{V}_0(r') \frac{\delta g_0(r)}{\delta u(r')} d\vec{r}', \quad (49)$$

so that Eq. (48) becomes

$$\frac{\hbar^2 \nabla^2 g_0(r)}{4m} = \int \tilde{V}_0(r') \frac{\delta g_0(r)}{\delta u(r')} d\vec{r}'. \quad (50)$$

Thus a sufficient condition for the variational condition [Eq. (44)] to be equivalent to the paired-pho-

non optimization condition [Eq. (50)] is that the functional derivative of $g(r)$ with respect to $u(r')$ be symmetric under interchange¹² and r' :

$$\delta g(r)/\delta u(r') = \delta g(r')/\delta u(r) . \quad (51)$$

A useful observation for generating approximations which satisfy this self-consistency condition is that it is satisfied for *any* approximation which can be expressed as an approximation for the normalization integral:

$$I = \int \prod_{i < j} e^{u(r_{ij})} d\vec{r}_1, \dots, d\vec{r}_N . \quad (52)$$

This is seen by noting that $g(r)$ is generated by the functional derivative of $\ln I$:

$$g(r) = \rho^{-2} \delta \ln I / \delta u(r) , \quad (53)$$

and consequently

$$\begin{aligned} \delta g(r)/\delta u(r') &= \rho^{-2} \delta^2 \ln I / \delta u(r') \delta u(r) \\ &= \delta g(r')/\delta u(r) . \end{aligned} \quad (54)$$

This gives a restriction which should be imposed upon any approximation used in conjunction with the paired-phonon analysis. Stated in terms of the fictitious classical system, the radial distribution function should be proportional to the functional derivative of the logarithm of the partition function with respect to the classical potential.²¹ Of course the exact relationship between $g(r)$ and $u(r)$ satisfies Eq. (53), which reaffirms our previous demonstration¹⁰ that the paired-phonon analysis optimization condition is equivalent to the variational extremum condition in the Jastrow function space.

It was noted in Ref. 10 that the HNC approximation is an approximation for which these two conditions are equivalent, while the PY approximation is not. This is easy to demonstrate in terms of Eq. (51). These two approximations are¹⁹ (HNC)

$$g(r) = e^{u(r)+P(r)} \quad (55)$$

and (PY)

$$g(r) = e^{u(r)[1+P(r)]} , \quad (56)$$

where $P(r)$ depends upon $g(r)$ through the liquid-structure function:

$$P(r) = \frac{1}{(2\pi)^3 \rho} \int e^{-i\vec{k}\cdot\vec{r}} \frac{[S(k)-1]^2}{S(k)} d\vec{k} , \quad (57)$$

$$S(k) - 1 = \rho \int [g(r) - 1] e^{i\vec{k}\cdot\vec{r}} d\vec{r} . \quad (58)$$

For these two approximations it is simpler to investigate $\delta u(r)/\delta g(r')$, which should also be symmetric in \vec{r} and \vec{r}' by Eq. (51). The results are (HNC)

$$\frac{\delta u(r)}{\delta g(r')} = \frac{\delta(\vec{r} - \vec{r}')}{g(r)} + \frac{1}{(2\pi)^3} \int e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} \left(\frac{1}{S(k)^2} - 1 \right) d\vec{k} \quad (59)$$

and (PY)

$$\begin{aligned} \frac{\delta u(r)}{\delta g(r')} &= \frac{\delta(\vec{r} - \vec{r}')}{g(r)} + \frac{1}{1+P(r)} \frac{1}{(2\pi)^3} \\ &\times \int e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} \left(\frac{1}{S(k)^2} - 1 \right) d\vec{k} . \end{aligned} \quad (60)$$

Equation (59) is symmetric under interchange of \vec{r} and \vec{r}' , but Eq. (60) is not because of the $P(r)$ in the denominator of the second term. Consequently the paired-phonon analysis provides a predictor-corrector procedure for determining the best Jastrow function within the HNC approximation, while it does not within the PY approximation. A similar analysis shows that the BBGKY-KSA approximation is not self-consistent in the present sense. We have not investigated the more complicated approximations such as improvements upon HNC and PY. In the remainder of this section we will restrict our attention to the HNC approximation.

To determine the paired-phonon analysis function $\mathcal{H}(k)$ within the HNC approximation, the function $u_0(r, \alpha)$ [Eq. (47)] is substituted for $u(r)$ in Eq. (55), so that $g(r) = g_0(r, \alpha)$. Then both sides of Eq. (55) are differentiated with respect to α and Fourier transformed to give $\mathcal{H}(k)$ in accord with Eq. (46). Since the right-hand side of Eq. (55) depends upon $g(r)$, the equation obtained for $\mathcal{H}(k)$ is a linear integral equation¹⁰

$$\begin{aligned} \frac{\mathcal{H}(k)}{S_0(k)^2} &= \bar{v}_0(k) + \frac{1}{(2\pi)^3 \rho} \int [1 - S_0(\vec{k} + \vec{h})] \\ &\times [1 - S_0(h)^2] \frac{\mathcal{H}(h)}{S_0(h)^2} d\vec{h} , \end{aligned} \quad (61)$$

where

$$\bar{v}_0(k) = \rho \int e^{i\vec{k}\cdot\vec{r}} g(r) \bar{V}_0(r) d\vec{r} .$$

We now give the details of the solution of this optimization problem within the HNC approximation at a single density (experimental equilibrium, $\rho = 0.02185 \text{ \AA}^{-3}$) and a single potential, the Lennard-Jones 6-12 potential with the de Boer-Michels parameters [see Eq. (63) below]. We follow the iterative procedure described at the end of Sec. II, i.e., we begin with a reasonable initial $u_0(r)$ from which we calculate $g_0(r)$, E_0/N , and $S_0(k)$ through Eqs. (55), (39), and (58), respectively, and $\mathcal{H}(k)$, ΔE_0 , and $\Delta u_0(r)$ through Eqs. (61), (27), (13), and (31). The entire procedure is then iterated with the new initial function $u_1(r) = u_0(r) + \Delta u_0(r)$, repeating the iteration until the minimization condition, Eq. (36), is satisfied. We examine

the sensitivity of the final result of this procedure to the initial $u_0(r)$ by using two different initial functions, one with $u_0(r) = -2(2.62/r)^5$, the other with $u_0(r) = -2(2.5/r)^6$. The energy as a function of iteration number is shown in Table I. In that table, E_n is calculated directly from u_n through Eqs. (39) and (55), and is not identical with the paired-phonon estimate, $E_{n-1} + \Delta E_{n-1}$. The difference is due in part to the approximation in Eq. (26) and in part due to the numerical integrations. The former error shrinks rapidly as the iterations converge, while the latter error should be of roughly the same order of magnitude for all iterations.

The final results for E , $g(r)$, and $S(k)$ all agree to within 1.5%. Figure 1 shows each initial $u_0(r)$ and the final $u(r)$. $u(r)$ is tabulated in column 4 of Table VI. The final $S(k)$ is plotted as the dashed line in Fig. 2 and tabulated in Column 2 of Table II, and the final $g(r)$ is tabulated in column 4 of Table IV. This calculation provides a good example of the insensitivity of the optimal wave function to the starting function of the iterative procedure.

In an independent calculation Shen *et al.*²² have demonstrated the same feature in a paired-phonon analysis optimization of the ground state of ${}^4\text{He}$ in two dimensions and the ground state of "homework" neutron star matter. Their starting functions appear to differ from one another by more than ours, so their test of the paired-phonon analysis is stronger than ours. The agreement between their final results is not as good as we have obtained here, but the agreement would undoubtedly improve with more iterations. It should be noted, however, that they obtain the energy by summing the predicted energy shifts E_n , rather than recomputing the energy at the end of each iteration.²³

TABLE I. Iterations of the paired-phonon analysis to obtain the ground-state energy of liquid ${}^4\text{He}$ at density 0.02185 \AA^{-3} in a Jastrow function using the HNC approximation. Column A begins with the Jastrow function defined by $u_0(r) = -2(2.62/r)^5$, while column B begins with $u_0(r) = -2(2.5/r)^6$. E_n is the calculated energy; ΔE_n is the paired-phonon analysis estimated shift.

	A	B		B	
	(°K)	(°K)	A	(°K)	
E_0	-4.414	-4.205	E_4	...	-4.542
ΔE_0	-0.204	-0.351	ΔE_4	...	-0.002
E_1	-4.609	-4.522	E_5	...	-4.549
ΔE_1	-0.004	-0.015	ΔE_5	...	-0.002
E_2	-4.615	-4.527	E_6	...	-4.549
ΔE_2	-0.001	-0.004	ΔE_6	...	-0.002
E_3	-4.617	-4.540	E_7	...	-4.552
ΔE_3	...	-0.003			

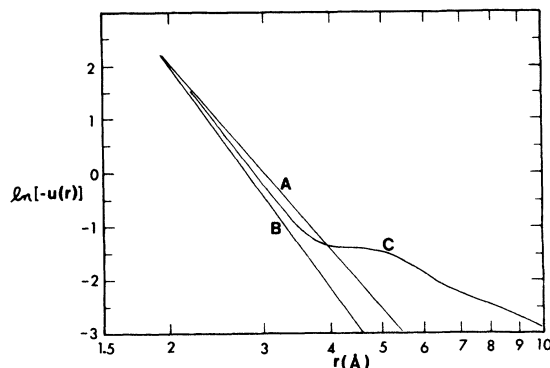


FIG. 1. Optimum Jastrow function [Eq. (4)] for liquid ${}^4\text{He}$ at the experimental equilibrium density $\rho_0 = 0.02185 \text{ \AA}^{-3}$ (curve C) compared to two different initial Jastrow functions for the paired-phonon analysis iterations: curve A, $u(r) = -2(2.62 \text{ \AA}/r)^5$; curve B, $u(r) = -2(2.5 \text{ \AA}/r)^6$.

Returning to our calculation as summarized in Table I, we note the rapid convergence with iteration number. The choice of $u_0(r)$ which converges most rapidly (three iterations) is the choice of the form of Eq. (6) with variationally determined parameters. The fact that the power in that $u_0(r)$ is 5 corresponds to the r^{-12} core of the Lennard-Jones potential. The rate of convergence of the $P=6$ choice may reflect the fact that the difference between $P=5$ and $P=6$ can be corrected only approximately by a finite sequence of Fourier transforms $\Delta u(r)$. That observation is given some support by the results of our calculation with another potential

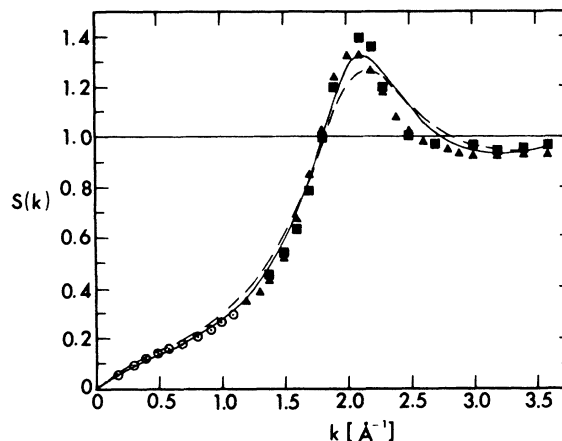


FIG. 2. Liquid-structure function of liquid ${}^4\text{He}$ at experimental equilibrium density $\rho_0 = 0.02185 \text{ \AA}^{-3}$; \odot , x-ray scattering at $T = 0.38 \text{ K}$ (Ref. 28); \blacktriangle , x-ray scattering at $T = 1.1 \text{ K}$ (Ref. 29); \blacksquare , neutron scattering at $T = 1.1 \text{ K}$ (Ref. 30); dashed line, from the optimum Jastrow function using the Lennard-Jones potential (Fig. 3); and solid line, from the optimum Jastrow function using the MDD-2 potential (Fig. 3).

TABLE II. Liquid-structure function $S(k)$ calculated for the ground state of ${}^4\text{He}$ at several different densities using the Lennard-Jones potential of Fig. 3. $S_J(k)$ is obtained from the optimum Jastrow trial function [Eq. (4)] within the HNC approximation. $\hat{S}(k)$ includes the effect of three-body factors in the ground-state wave function [Eq. (65)]. The wave number scale is in units of λ^{-1} , where $\lambda = (\rho/\rho_0)^{1/3}$.

$\lambda^{-1}k(\text{\AA}^{-1}) \backslash \rho(\text{\AA}^{-3})$	0.021 85		0.023 88		0.025 71		0.028 44	
	$S_J(k)$	$\hat{S}(k)$	$S_J(k)$	$\hat{S}(k)$	$S_J(k)$	$\hat{S}(k)$	$S_J(k)$	$\hat{S}(k)$
0.1	0.039	0.037	0.032	0.031	0.028	0.027	0.024	0.023
0.2	0.072	0.068	0.061	0.057	0.053	0.050	0.045	0.042
0.3	0.101	0.093	0.086	0.080	0.076	0.071	0.065	0.060
0.4	0.126	0.115	0.110	0.100	0.098	0.090	0.085	0.078
0.5	0.150	0.136	0.133	0.120	0.120	0.109	0.105	0.095
0.6	0.174	0.158	0.156	0.141	0.142	0.129	0.125	0.113
0.8	0.227	0.207	0.207	0.189	0.192	0.175	0.172	0.157
1.0	0.295	0.275	0.274	0.255	0.257	0.240	0.235	0.219
1.2	0.388	0.371	0.367	0.351	0.349	0.334	0.323	0.311
1.4	0.523	0.517	0.505	0.501	0.488	0.487	0.464	0.465
1.6	0.718	0.738	0.710	0.736	0.700	0.732	0.685	0.724
1.8	0.974	1.040	0.997	1.081	1.018	1.121	1.048	1.183
1.9	1.103	1.190	1.142	1.254	1.179	1.318	1.239	1.424
2.0	1.204	1.303	1.247	1.372	1.287	1.440	1.348	1.548
2.1	1.256	1.348	1.297	1.410	1.335	1.469	1.390	1.560
2.2	1.258	1.330	1.290	1.374	1.318	1.415	1.357	1.473
2.3	1.225	1.271	1.239	1.288	1.248	1.299	1.256	1.310
2.4	1.176	1.200	1.174	1.195	1.168	1.187	1.155	1.170
2.6	1.077	1.074	1.063	1.056	1.050	1.038	1.029	1.011
2.8	1.005	0.992	0.988	0.972	0.973	0.953	0.951	0.926
3.0	0.963	0.950	0.949	0.934	0.938	0.921	0.921	0.902
3.2	0.946	0.936	0.937	0.926	0.929	0.918	0.919	0.908
3.4	0.947	0.942	0.943	0.938	0.941	0.936	0.939	0.935
3.6	0.960	0.958	0.961	0.961	0.964	0.965	0.969	0.972
3.8	0.978	0.980	0.984	0.987	0.989	0.994	0.999	1.007
4.0	0.996	0.999	1.003	1.008	1.010	1.017	1.021	1.029
4.2	1.009	1.013	1.015	1.020	1.021	1.026	1.028	1.034
4.4	1.015	1.018	1.020	1.023	1.023	1.026	1.026	1.029
4.6	1.016	1.018	1.017	1.019	1.017	1.018	1.016	1.016
4.8	1.013	1.013	1.012	1.012	1.010	1.010	1.007	1.005
5.0	1.008	1.007	1.005	1.004	1.002	1.001	0.998	0.996

in Sec. IV. In that case the short-range behavior of the optimum $u(r)$ is not r^{-5} , so even beginning with the optimum $u_0(r)$ of the form of Eq. (6), it still takes seven iterations to obtain the same convergence.

IV. OPTIMUM JASTROW FUNCTION AT SEVERAL DENSITIES

In this section we calculate the liquid-structure function and energy expectation value in the optimum Jastrow function as a function of density. We use a reference procedure to correct approximately the systematic error caused by the HNC approximation.²⁴ The procedure is to first obtain the density dependence of the optimum energy E_0^{HNC} from the simple parametrized form, $u_0(r) = -(b/r)^5$, within the HNC approximation, and then apply the self-consistent paired-phonon analysis to this

result to obtain the optimal HNC energy $E_{\text{OPT}}^{\text{HNC}}$. The energy shift $E_J = E_{\text{OPT}}^{\text{HNC}} - E_0^{\text{HNC}}$ is then added to the optimized Monte Carlo or molecular-dynamics energy E_0^{MC} based upon the same parametrization, giving our estimate of the optimum Jastrow energy as

$$E_J = E_0^{\text{MC}} + (E_{\text{OPT}}^{\text{HNC}} - E_0^{\text{HNC}}). \quad (62)$$

The self-consistent paired-phonon calculation is done at the following densities: $\rho = 0.01796$, 0.01946 , 0.02096 , 0.02185 , 0.02388 , and 0.02571 (\AA^{-3}). Two different interaction potentials are used²⁵: the Lennard-Jones 6-12 potential

$$V(r) = 4\epsilon [(\sigma/r)^{12} - (\sigma/r)^6], \quad (63)$$

$$\epsilon = 10.22 \text{ (K)}, \quad \sigma = 2.556 \text{ (\AA)},$$

and the second Morse-dipole-dipole potential (MDD-2) of Bruch and McGee.^{25,26}

$$V(r) = \begin{cases} 1.987047 \times 10^6 \exp(-3.4573r - 0.26206r^2)(K); & r < 0.8919 \text{ \AA}, \\ 10.7498 \{ \exp[2c(1-x)] - 2 \exp[c(1-x)] \} (K); & 0.8919 < r < 3.682 \text{ \AA}, \\ -10^4(1.021376/r^6 + 2.767132/r^8) (K); & y > 3.682 \text{ \AA}, \end{cases} \quad (64)$$

where

$$c = 6.127768, \quad \chi = r/3.0238 \text{ \AA}.$$

These potentials are compared in Fig. 3. The energies obtained in these calculations are tabulated in the first six columns of Tables VIII and IX. Results are also given for the Lennard-Jones potential at $\rho = 0.02844 \text{ \AA}^{-3}$, the lowest density of solid ^4He . The Monte Carlo results for both potentials used here are those obtained by Murphy and Watts.⁶ The optimum Jastrow energy as a function of density is compared to the Monte Carlo result and experiment in Fig. 4, where it can be seen that the optimum Jastrow energies obtained by such a reference procedure give a better agreement with experiment than the parametrized Monte Carlo energies. Both the equilibrium density and the magnitude of the energy obtained from the Lennard-Jones potential agree better with experiment than the same quantities calculated with MDD-2 potential.

The results of our Jastrow calculation of the liquid-structure function are shown in Fig. 2 at equilibrium density and in the columns labeled S_r

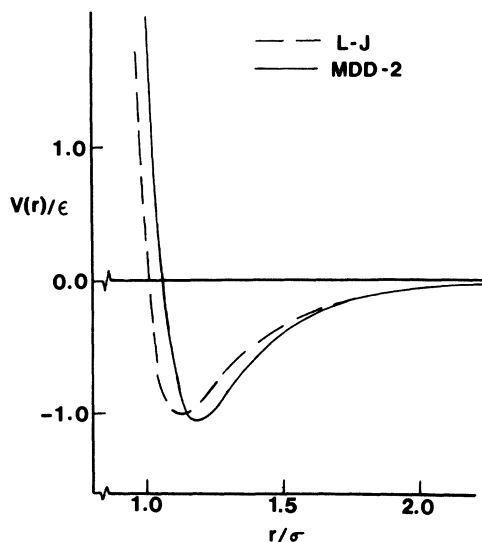


FIG. 3. Two candidates for the interaction between two helium atoms: dashed line, the Lennard-Jones 6-12 potential; and solid line, the MDD-2 potential (Ref. 25). r is in units of $\sigma = 2.556 \text{ \AA}$, and $V(r)$ is in units of $\epsilon = 10.22 \text{ K}$.

in Tables II and III as a function of density. We have used no reference procedure to correct for the HNC approximation for $S(k)$ since the relative errors are much smaller than in the energy calculation discussed above. Except for long wavelengths, the HNC approximation differs from the

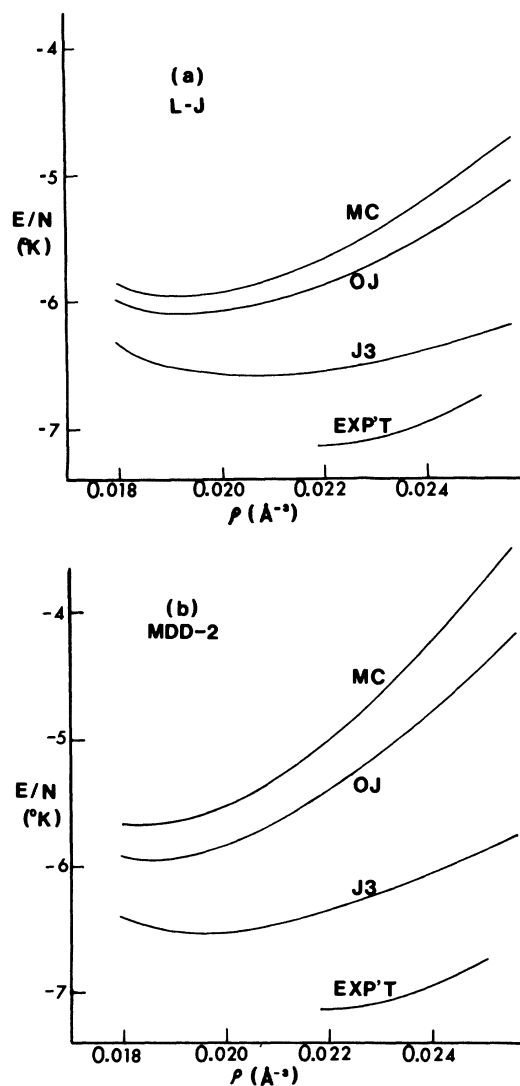


FIG. 4. Energy per particle as a function of density for (a) the Lennard-Jones potential; and (b) the MDD-2 potential. Curve MC, the parametrized Monte Carlo calculation of Ref. 6; OJ, the optimized Jastrow result of Sec. IV; J3, the result including three-body factors (Sec. V); and EXP'T, the experimental results.

TABLE III. Liquid-structure function $S(k)$ as in Table II, but using the MDD-2 potential of Fig. 3. Note that there are only three common densities with Table II, and the wave-number scale is changed.

k (\AA^{-1})	ρ (\AA^{-3})		0.019 46		0.021 85		0.023 88		0.025 71	
	$S_J(k)$	$\hat{S}(k)$	$S_J(k)$	$\hat{S}(k)$	$S_J(k)$	$\hat{S}(k)$	$S_J(k)$	$\hat{S}(k)$	$S_J(k)$	$\hat{S}(k)$
0.1	0.043	0.042	0.032	0.031	0.026	0.025	0.022	0.022		
0.2	0.081	0.076	0.061	0.058	0.051	0.048	0.044	0.041		
0.3	0.112	0.103	0.087	0.081	0.073	0.068	0.064	0.059		
0.4	0.138	0.126	0.111	0.101	0.094	0.086	0.083	0.075		
0.5	0.163	0.148	0.134	0.121	0.115	0.104	0.101	0.092		
0.6	0.188	0.170	0.157	0.142	0.136	0.122	0.120	0.109		
0.8	0.244	0.224	0.208	0.189	0.182	0.165	0.163	0.148		
1.0	0.317	0.296	0.272	0.253	0.241	0.223	0.216	0.200		
1.2	0.419	0.403	0.363	0.348	0.322	0.307	0.291	0.276		
1.4	0.568	0.566	0.497	0.493	0.443	0.438	0.400	0.394		
1.6	0.786	0.814	0.702	0.728	0.632	0.654	0.573	0.591		
1.8	1.056	1.132	0.992	1.076	0.922	1.005	0.852	0.930		
1.9	1.174	1.266	1.145	1.261	1.096	1.223	1.036	1.163		
2.0	1.247	1.341	1.265	1.398	1.256	1.421	1.226	1.411		
2.1	1.264	1.339	1.316	1.436	1.351	1.519	1.368	1.581		
2.2	1.237	1.288	1.301	1.389	1.359	1.495	1.411	1.602		
2.3	1.188	1.214	1.247	1.297	1.306	1.390	1.367	1.494		
2.4	1.133	1.142	1.180	1.202	1.229	1.271	1.281	1.350		
2.6	1.038	1.030	1.059	1.051	1.083	1.078	1.109	1.109		
2.8	0.978	0.966	0.983	0.966	0.989	0.970	0.998	0.976		
3.0	0.949	0.938	0.943	0.928	0.940	0.920	0.938	0.915		
3.2	0.943	0.936	0.932	0.922	0.923	0.909	0.916	0.897		
3.4	0.953	0.950	0.941	0.936	0.930	0.922	0.919	0.909		
3.6	0.972	0.973	0.962	0.962	0.951	0.950	0.940	0.938		
3.8	0.992	0.995	0.986	0.990	0.979	0.983	0.970	0.974		
4.0	1.008	1.012	1.007	1.012	1.004	1.011	1.000	1.008		
4.2	1.016	1.019	1.019	1.024	1.020	1.027	1.021	1.030		
4.4	1.017	1.019	1.021	1.024	1.025	1.030	1.029	1.036		
4.6	1.013	1.014	1.017	1.019	1.022	1.024	1.026	1.030		
4.8	1.007	1.007	1.010	1.010	1.014	1.014	1.018	1.018		
5.0	1.002	1.001	1.003	1.002	1.005	1.004	1.008	1.006		

Monte Carlo calculation of $S(k)$ for the same $u(r)$ by only a few percent.²⁷ In particular, the maximum in $S(k)$ is 1% less in the HNC calculation than in the Monte Carlo calculation for the parametrized $u(r)$ of Eq. (6) with parameters chosen to minimize the Monte Carlo energy. The reason that the HNC approximation works so well for $S(k)$ is that the error it makes is greatest when $u(r)$ is large, which is where $g(r)$ is small and thus contributes little to $S(k)$. Both the potential and kinetic energy have large contributions from this region, so they are in larger error. Furthermore, the minimization of the energy with respect to the parameters in $u(r)$ produces a value of b greater by 1% than the value obtained in the Monte Carlo calculation. Consequently the small discrepancy between the HNC and Monte Carlo $S(k)$ is reduced by comparing the $S(k)$'s at their respective optimum values of b . Our conclusion is that the HNC calculation of $S(k)$ is a very good approximation to the result that would be obtained by the Monte Carlo calculation.

tion.

The calculated $S(k)$ at equilibrium density using each interaction is compared with x-ray and neutron scattering results in Fig. 2. The long-wavelength x-ray scattering is at a temperature of 0.38 °K,²⁸ the intermediate-wavelength x-ray measurements are at 0.79 °K,²⁹ and the neutron scattering results are at 1.1 °K.³⁰ The calculation using the MDD-2 potential is in slightly better agreement with experiment than the one using the Lennard-Jones potential, although both have a broader first maximum than experiment. From Tables II and III it can be seen that the peak in the calculated $S(k)$ increases in magnitude and moves to larger values of k with increasing density. Experimental neutron scattering results have the same qualitative behavior,³¹ but, as can be seen in Fig. 5(a), the quantitative agreement of the density dependence of the calculated and observed $S(k)$ is not good. It should be noted, however, that the experiment was done at a somewhat elevated tempera-

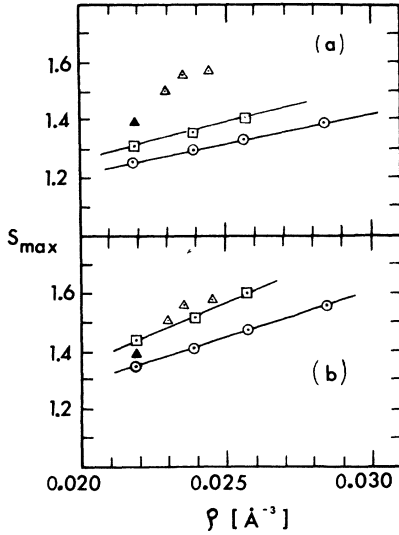


FIG. 5. Maximum value of the liquid-structure function as a function of density. (a) Obtained from the optimum Jastrow function; (b) the effects of three-body factors. The experimental points are from neutron scattering; \blacktriangle , $T = 1.1^\circ\text{K}$ (Ref. 30); and \triangle , $T = 2.05, 2.02,$ and 1.94°K with increasing density (Ref. 31). The ground-state calculation is for the Lennard-Jones potential (\odot) and the MDD-2 potential (\square) at the densities indicated by the points. The lines are to aid the eye only.

ture (about 2°K). Mozer *et al.* also obtained data at a higher temperature and found that the peak value increases with increasing temperature,³¹ which may also explain the discrepancy between the x-ray and neutron scattering data in Fig. 2. We speculate therefore that the density dependence of $S(k)$ measured at much lower temperatures would be in better agreement with the calculations described in this section.

The results of our Jastrow calculation of the radial distribution function $g(r)$ are tabulated in Tables IV and V. Note that the maximum value of $g(r)$ increases with increasing density, while the position of the maximum decreases. This peak is located at smaller r for the MDD-2 interaction than

for the Lennard-Jones interaction, in spite of the fact that the minimum value of the latter interaction is at smaller r . On the other hand, the maximum value of $g(r)$ is larger for the MDD-2 potential as one might expect from its greater depth.

The optimum $u(r)$ for the Jastrow trial function is tabulated in Tables VI and VII. Note that there is some structure in $u(r)$ similar to that seen in Fig. 1, including an inflection near the peak position in $g(r)$ which develops into a maximum at higher density. Nowhere, however, does $u(r)$ come close to changing signs and becoming positive in contrast to a recent suggestion that a positive maximum is necessary for a self-bound system.³²

V. EXTENDED JASTROW CALCULATION

The results of the optimal Jastrow calculation for the ground-state energy may be improved upon by considering an expanded space of trial functions of the form of Eqs. (7) and (8).¹³⁻¹⁵ To find the optimal wave function in this enlarged space we use the general optimization procedure for extended Jastrow functions developed elsewhere.¹⁴ For a practical calculation we first set $u_n = 0$ for $n \geq 3$ and use the optimum u_2 obtained in Sec. IV. We then vary u_3 with $u_n = 0$ for $n \geq 4$. Then the trial function has the form

$$\hat{\Psi}(\vec{r}_1, \dots, \vec{r}_N) = \Psi_J(\vec{r}_1, \dots, \vec{r}_N) \times \exp\left(\frac{1}{2} \sum_{i \neq j \neq k} \frac{1}{3!} u_3(\vec{r}_i, \vec{r}_j, \vec{r}_k)\right), \quad (65)$$

where $\hat{\Psi}_J$ is the optimum Jastrow wave function and thus satisfies Eq. (36). The variational procedure takes on a simple form when $u_3(r_1, r_2, r_3)$ is expressed in terms of its Fourier transform:

$$u_3(\vec{r}_1, \vec{r}_2, \vec{r}_3) = N^{-2} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3} c_3(\vec{k}_1, \vec{k}_2, \vec{k}_3) \prod_{i=1}^3 e^{i\vec{k}_i \cdot \vec{r}_i}. \quad (66)$$

Then the wave function Ψ becomes

$$\Psi(\vec{r}_1, \dots, \vec{r}_N) = \Psi_J(\vec{r}_1, \dots, \vec{r}_N) \exp\left(\frac{1}{2N^2} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3} \rho^{(3)}(\vec{k}_1, \vec{k}_2, \vec{k}_3) c_3(\vec{k}_1, \vec{k}_2, \vec{k}_3)\right), \quad (67)$$

where

$$\rho^{(3)}(\vec{k}_1, \vec{k}_2, \vec{k}_3) = \sum_{i_1 \neq i_2 \neq i_3}^N e^{i(\vec{k}_1 \cdot \vec{r}_{i_1} + \vec{k}_2 \cdot \vec{r}_{i_2} + \vec{k}_3 \cdot \vec{r}_{i_3})}. \quad (68)$$

The energy is then minimized with respect to $c_3(k_1, k_2, k_3)$. The results obtained in Ref. 14 are

$$c_3(\vec{k}_1, \vec{k}_2, \vec{k}_3) = -[\mathcal{N}(\vec{k}_1, \vec{k}_2, \vec{k}_3) / \mathcal{D}(\vec{k}_1, \vec{k}_2, \vec{k}_3)] \delta_{\vec{k}_1 + \vec{k}_2 + \vec{k}_3, 0}, \quad (69)$$

TABLE IV. Radial distribution function $g(r)$ calculated for the ground state of ${}^4\text{He}$ at several different densities using the Lennard-Jones potential of Fig. 3. $g(r)$ is obtained from the optimum Jastrow trial function [Eq. (4)] within the HNC approximation. The length scale of the last three columns is $\lambda = (\rho/\rho_0)^{1/3}$, $\rho_0 = 0.02185 \text{ \AA}^{-3}$.

$r \text{ (\AA)} \backslash \rho \text{ (\AA}^{-3}\text{)}$	0.01946	0.02096	0.02185	$r\lambda \text{ (\AA)}$	0.02388	0.02571	0.02844
1.8	0.4×10^{-4}	0.4×10^{-4}	0.4×10^{-4}	1.8	0.2×10^{-4}	0.1×10^{-4}	0.6×10^{-5}
1.9	0.6×10^{-3}	0.7×10^{-3}	0.7×10^{-3}	1.9	0.4×10^{-3}	0.2×10^{-3}	0.1×10^{-3}
2.0	0.005	0.005	0.005	2.0	0.003	0.002	0.1×10^{-2}
2.1	0.022	0.025	0.025	2.1	0.016	0.010	0.005
2.2	0.065	0.072	0.073	2.2	0.049	0.032	0.017
2.3	0.145	0.158	0.164	2.3	0.116	0.081	0.048
2.4	0.261	0.283	0.294	2.4	0.223	0.170	0.110
2.5	0.407	0.437	0.455	2.5	0.370	0.303	0.218
2.6	0.566	0.605	0.628	2.6	0.544	0.472	0.373
2.7	0.726	0.772	0.799	2.7	0.726	0.660	0.562
2.8	0.874	0.924	0.953	2.8	0.898	0.844	0.760
2.9	1.001	1.052	1.082	2.9	1.046	1.009	0.947
3.0	1.103	1.151	1.180	3.0	1.165	1.146	1.111
3.1	1.177	1.221	1.247	3.1	1.252	1.251	1.243
3.2	1.227	1.264	1.287	3.2	1.307	1.323	1.339
3.3	1.254	1.285	1.304	3.3	1.335	1.362	1.397
3.4	1.264	1.287	1.302	3.4	1.339	1.373	1.420
3.5	1.259	1.275	1.286	3.5	1.326	1.362	1.417
3.6	1.243	1.253	1.259	3.6	1.299	1.337	1.393
3.7	1.220	1.224	1.225	3.7	1.264	1.301	1.357
3.8	1.192	1.190	1.188	3.8	1.224	1.259	1.311
3.9	1.162	1.155	1.150	3.8	1.182	1.212	1.259
4.0	1.130	1.120	1.112	4.0	1.139	1.165	1.204
4.2	1.069	1.054	1.044	4.2	1.060	1.076	1.100
4.4	1.017	1.000	0.989	4.4	0.996	1.003	1.014
4.6	0.977	0.961	0.950	4.6	0.949	0.948	0.948
4.8	0.951	0.937	0.928	4.8	0.920	0.913	0.903
5.0	0.938	0.928	0.921	5.0	0.909	0.898	0.882
5.2	0.937	0.931	0.928	5.2	0.913	0.900	0.880
5.4	0.945	0.944	0.943	5.4	0.929	0.915	0.894
5.6	0.959	0.961	0.964	5.6	0.952	0.940	0.921
5.8	0.975	0.980	0.985	5.8	0.977	0.969	0.955
6.0	0.990	0.998	1.003	6.0	1.000	0.996	0.988
6.2	1.003	1.011	1.016	6.2	1.018	1.018	1.018

where

$$\begin{aligned} \mathcal{H}(\vec{k}_1, \vec{k}_2, \vec{k}_3) = & -(\hbar^2/8m)(k_1^2 + k_2^2 + k_3^2)S(k_1)S(k_2)S(k_3) + (\hbar^2/8m)(k_1^2 - k_2^2 - k_3^2)S(k_1) \\ & + (\hbar^2/8m)(k_2^2 - k_1^2 - k_3^2)S(k_2) + (\hbar^2/8m)(k_3^2 - k_1^2 - k_2^2)S(k_3) \\ & + (\hbar^2/4m)[k_1^2/S(k_1) + k_2^2/S(k_2) + k_3^2/S(k_3)]S(k_1)S(k_2)S(k_3) \end{aligned} \quad (70)$$

and

$$\mathcal{D}(\vec{k}_1, \vec{k}_2, \vec{k}_3) = (\hbar^2/4m)(k_1^2/S(k_1) + k_2^2/S(k_2) + k_3^2/S(k_3))S(k_1)S(k_2)S(k_3). \quad (71)$$

The convolution approximation for the three-body structure factor

$$\langle \Psi | \rho_{\vec{k}_1}^\dagger \rho_{\vec{k}_2}^\dagger \rho_{\vec{k}_3}^\dagger | \Psi \rangle \simeq \delta_{\vec{k}_1 + \vec{k}_2 + \vec{k}_3, 0} N S(k_1) S(k_2) S(k_3) \quad (72)$$

has been used in these results.¹ The shift in energy obtained in this manner is

$$\delta E_3 = \frac{-1}{3!} \frac{1}{2N} \sum_{\substack{\vec{k}_1, \vec{k}_2, \vec{k}_3 \\ \vec{k}_3 + \vec{k}_2 + \vec{k}_1 = 0}} \frac{\mathcal{H}(\vec{k}_1, \vec{k}_2, \vec{k}_3)}{\mathcal{D}(\vec{k}_1, \vec{k}_2, \vec{k}_3)}. \quad (73)$$

TABLE V. Radial distribution function $g(r)$ calculated for the ground state of ${}^4\text{He}$ at several different densities using the MDD-2 potential of Fig. 3. $g(r)$ is obtained from the optimum Jastrow trial function [Eq. (4)] within the HNC approximation. Note that there are five densities in common with Table IV but the length scale is changed.

r (Å) \ ρ (Å ⁻³)	0.017 96	0.019 46	0.020 96	0.021 85	0.023 88	0.025 71
1.8	0.5×10^{-5}	0.5×10^{-5}	0.5×10^{-5}	0.5×10^{-5}	0.6×10^{-5}	0.8×10^{-5}
1.9	0.1×10^{-3}	0.1×10^{-3}	0.2×10^{-3}	0.2×10^{-3}	0.2×10^{-3}	0.3×10^{-3}
2.0	0.002	0.002	0.002	0.002	0.002	0.003
2.1	0.009	0.010	0.011	0.012	0.015	0.017
2.2	0.032	0.036	0.039	0.043	0.051	0.059
2.3	0.083	0.092	0.100	0.109	0.126	0.143
2.4	0.167	0.183	0.200	0.213	0.242	0.272
2.5	0.284	0.308	0.335	0.352	0.395	0.438
2.6	0.426	0.459	0.496	0.517	0.575	0.631
2.7	0.582	0.624	0.670	0.698	0.768	0.835
2.8	0.742	0.792	0.845	0.877	0.956	1.029
2.9	0.892	0.947	1.003	1.038	1.119	1.193
3.0	1.023	1.078	1.134	1.168	1.246	1.314
3.1	1.127	1.180	1.233	1.263	1.332	1.391
3.2	1.204	1.251	1.298	1.324	1.382	1.429
3.3	1.254	1.295	1.334	1.356	1.401	1.434
3.4	1.282	1.315	1.346	1.363	1.394	1.415
3.5	1.290	1.315	1.337	1.349	1.367	1.375
3.6	1.282	1.300	1.313	1.319	1.325	1.322
3.7	1.263	1.273	1.279	1.279	1.275	1.262
3.8	1.236	1.239	1.238	1.235	1.221	1.202
3.9	1.205	1.202	1.196	1.189	1.169	1.144
4.0	1.171	1.164	1.153	1.144	1.119	1.091
4.2	1.104	1.090	1.072	1.060	1.029	0.999
4.4	1.043	1.025	1.005	0.991	0.960	0.931
4.6	0.994	0.975	0.955	0.943	0.915	0.891
4.8	0.959	0.942	0.924	0.914	0.892	0.875
5.0	0.938	0.923	0.910	0.902	0.888	0.879
5.2	0.930	0.920	0.911	0.907	0.902	0.901
5.4	0.933	0.928	0.925	0.925	0.928	0.935
5.6	0.944	0.944	0.946	0.949	0.959	0.973
5.8	0.960	0.964	0.971	0.976	0.991	1.008
6.0	0.978	0.985	0.995	1.001	1.019	1.036
6.2	0.995	1.003	1.014	1.020	1.036	1.050

The new liquid-structure factor $S(k)$ becomes

$$\hat{S}(k) = S(k) \exp \left(\frac{-S(k)}{2N} \sum_{\dagger} [S(\vec{k} + \vec{l})S(l) - 1] \frac{\alpha(\vec{k}, \vec{l}, -\vec{k} - \vec{l})}{\alpha(\vec{k}, \vec{l}, -\vec{k} - \vec{l})} \right). \quad (74)$$

The numerical calculation is done at the same densities and potentials as in Sec. IV. Adding the optimum Jastrow energy obtained by the reference procedure described in Sec. IV to the energy shift from the three-body extended Jastrow factors found here gives us our final estimate of the ground-state energy as a function of density. The numerical results for the energy are given in the last two columns of Tables VIII and IX and are plotted in Fig. 4. As in the previous calculation at equilibrium density,¹⁴ we find that the three-body factors make a significant contribution to the energy, improving

agreement with experiment over the Jastrow result. We also find, as should be expected, that the three-body factors have increasing importance as the density is increased. Consequently the calculated equilibrium density is closer to the experimental value. As in the Jastrow calculation in Sec. IV, both the equilibrium density and the magnitude of the energy obtained using the Lennard-Jones potential agree better with experiment than the same quantities calculated with the MDD-2 potential.

The liquid-structure function at equilibrium density is compared to the experimental values in Fig.

TABLE VI. Function $-u(r)$ for the optimum Jastrow function of the form

$$\prod_{i < j} e^{u(r_{ij})/2}$$

determined variationally within the HNC approximation using the Lennard-Jones potential of Fig. 3. The length scale of the last three columns is λ where $\lambda = (\rho/\rho_0)^{1/3}$, $\rho_0 = 0.02185 \text{ \AA}^{-3}$.

$r \text{ (\AA)} \backslash \rho_0 \text{ (\AA}^{-3}\text{)}$	0.01946	0.02096	0.02185	$r\lambda \text{ (\AA)}$	0.02388	0.02571	0.02844
1.8	12.269	12.353	12.712	1.8	13.608	14.533	15.848
1.9	9.297	9.380	9.628	1.9	10.494	11.385	12.656
2.0	7.136	7.217	7.387	2.0	8.221	9.070	10.293
2.1	5.540	5.620	5.737	2.1	6.526	7.319	8.477
2.2	4.347	4.425	4.507	2.2	5.233	5.951	7.019
2.3	3.443	3.518	3.579	2.3	4.224	4.853	5.807
2.4	2.749	2.821	2.868	2.4	3.424	3.958	4.783
2.5	2.209	2.276	2.315	2.5	2.784	3.229	3.924
2.6	1.783	1.844	1.879	2.6	2.270	2.639	3.218
2.7	1.443	1.499	1.530	2.7	1.857	2.166	2.647
2.8	1.170	1.221	1.249	2.8	1.527	1.788	2.191
2.9	0.951	0.999	1.025	2.9	1.261	1.483	1.824
3.0	0.775	0.820	0.845	3.0	1.047	1.236	1.526
3.1	0.634	0.678	0.701	3.1	0.875	1.036	1.283
3.2	0.522	0.565	0.587	3.2	0.736	0.874	1.085
3.3	0.433	0.476	0.496	3.3	0.627	0.746	0.927
3.4	0.363	0.405	0.426	3.4	0.540	0.644	0.802
3.5	0.308	0.351	0.371	3.5	0.473	0.565	0.703
3.6	0.266	0.309	0.330	3.6	0.422	0.504	0.626
3.7	0.234	0.278	0.300	3.7	0.383	0.456	0.566
3.8	0.210	0.255	0.278	3.8	0.354	0.421	0.520
3.9	0.193	0.239	0.263	3.9	0.334	0.396	0.487
4.0	0.182	0.228	0.253	4.0	0.320	0.379	0.465
4.2	0.170	0.217	0.243	4.2	0.306	0.360	0.439
4.4	0.168	0.215	0.241	4.4	0.301	0.352	0.428
4.6	0.168	0.214	0.240	4.6	0.299	0.350	0.425
4.8	0.168	0.212	0.237	4.8	0.295	0.346	0.421
5.0	0.166	0.206	0.229	5.0	0.286	0.336	0.410
5.2	0.160	0.197	0.218	5.2	0.272	0.321	0.393
5.4	0.151	0.184	0.202	5.4	0.254	0.301	0.371
5.6	0.140	0.169	0.185	5.6	0.234	0.277	0.342
5.8	0.128	0.154	0.168	5.8	0.212	0.252	0.311
6.0	0.116	0.139	0.152	6.0	0.192	0.228	0.282
6.2	0.105	0.126	0.138	6.2	0.174	0.206	0.254

6. The height of the maximum has increased over the value shown in Fig. 2 for the Jastrow calculation for both potentials. In contrast to the Jastrow calculation, the Lennard-Jones potential now seems to agree somewhat better with experiment than MDD-2. The fact that the width of the first peak in $S(k)$ is too large continues to be a problem.

The calculated liquid-structure function at several densities is shown in Fig. 7(a) for the Lennard-Jones potential and in Fig. 7(b) for the MDD-2 potential. It can be seen in Tables II and III and Fig. 5 that the contribution of three-body factors to $S(k)$ increases with density. The magnitude of the peak in $S(k)$ is compared to the experimental results in Fig. 5(b). Again the calculated density dependence seems poor, although we recall the discussion of

the same point in Sec. IV where we noted that the temperature effects on the finite pressure $S(k)$ may be partly responsible for the poor agreement.

VI. DISCUSSION

The calculation described in this paper gives an example of the sensitivity of the ground-state properties of liquid ${}^4\text{He}$ to the interaction potential. A reasonable objective for such a calculation is the determination of a density-independent interaction between helium atoms which reproduces the experimentally determined liquid-structure function and binding energy *for all densities*. Since the energy is sensitive to the short-range behavior of the potential and the structure function is sensitive to

TABLE VII. Function $-u(r)$ for the optimum Jastrow function of the form determined variationally within the HNC approximation using the MDD-2 potential of Fig. 3. Note that there are five densities in common with Table VI.

r (Å) \ ρ (Å ⁻³)	0.017 96	0.019 46	0.020 96	0.021 85	0.023 88	0.025 71
1.8	14.397	14.607	14.943	14.992	15.161	15.273
1.9	10.904	11.069	11.320	11.341	11.478	11.561
2.0	8.363	8.498	8.689	8.696	8.813	8.882
2.1	6.492	6.607	6.756	6.762	6.857	6.931
2.2	5.099	5.203	5.323	5.337	5.434	5.497
2.3	4.049	4.147	4.247	4.272	4.363	4.425
2.4	3.245	3.338	3.426	3.459	3.542	3.602
2.5	2.617	2.705	2.783	2.820	2.895	2.949
2.6	2.116	2.198	2.267	2.303	2.369	2.416
2.7	1.711	1.785	1.848	1.879	1.938	1.979
2.8	1.380	1.448	1.505	1.532	1.585	1.621
2.9	1.112	1.174	1.226	1.251	1.299	1.332
3.0	0.895	0.953	1.002	1.026	1.072	1.104
3.1	0.721	0.777	0.824	0.847	0.892	0.925
3.2	0.583	0.637	0.683	0.706	0.750	0.783
3.3	0.414	0.527	0.571	0.593	0.638	0.672
3.4	0.388	0.440	0.483	0.506	0.551	0.588
3.5	0.321	0.372	0.416	0.439	0.487	0.526
3.6	0.271	0.322	0.366	0.390	0.440	0.482
3.7	0.233	0.285	0.330	0.355	0.407	0.453
3.8	0.206	0.258	0.304	0.330	0.385	0.433
3.9	0.187	0.239	0.287	0.313	0.370	0.421
4.0	0.174	0.227	0.275	0.302	0.361	0.413
4.2	0.161	0.215	0.265	0.293	0.355	0.410
4.4	0.160	0.214	0.265	0.294	0.357	0.412
4.6	0.163	0.217	0.267	0.295	0.356	0.408
4.8	0.167	0.219	0.266	0.293	0.350	0.398
5.0	0.168	0.217	0.262	0.287	0.338	0.380
5.2	0.166	0.211	0.251	0.273	0.318	0.353
5.4	0.159	0.200	0.236	0.255	0.293	0.322
5.6	0.150	0.186	0.218	0.235	0.267	0.290
5.8	0.138	0.171	0.198	0.212	0.240	0.259
6.0	0.126	0.155	0.179	0.191	0.215	0.232
6.2	0.113	0.140	0.162	0.173	0.194	0.210

the intermediate and long-range behavior of the potential, that experimental information should be more than adequate to determine the interaction function. For the purpose of comparing to a ground state theory it would be very useful to have the finite-pressure liquid-structure function measured at a much lower temperature.

There are two requirements that the theory must meet in order to make use of the experimental data to determine the potential. The first is that the structure of the model Hamiltonian is adequate and the second is that the ground state of the model Hamiltonian can be solved accurately. Concerning the first requirement, in our calculations we have assumed that the fundamental interaction between helium atoms is a two-body interaction. Helium atoms however are not elementary particles, and consequently there are fundamental three-body and

higher interactions. Murphy and Barker have estimated that the contribution of the triple-dipole three body interactions to the ground-state energy per particle near equilibrium density is $0.14 (\rho/\rho_0)^3$ °K.³³ The short-range part of the potential is not known, but the amount it contributes should be small due to the suppression of the wave function at close approaches by the two-body potential. Thus the contribution to the energy per particle from n -body potentials with $n \geq 3$ is probably less than 0.2°K , and the density variation is probably less than 0.1°K over the range of experimental densities.

The question which remains is whether the theoretical calculation presented in this paper is adequate to sort out possible potentials. That is, have we solved the ground-state problem accurately? The extended Jastrow function is certainly not the

TABLE VIII. Energy terms for the estimate of the ground-state energy per particle of ${}^4\text{He}$ interacting by the Lennard-Jones potential of Eq. (63). $E_{\text{OPT}}^{\text{HNC}}$ is the variational extremum energy for the Jastrow function within the HNC approximation, E_0^{HNC} the minimum for the parametrization of Eq. (6), $\Delta E_J = E_{\text{OPT}}^{\text{HNC}} - E_0^{\text{HNC}}$, E_0^{MC} is the minimum for the parametrization of Eq. (6) calculated using the Monte Carlo integration (Ref. 6), and $E_J = E_0^{\text{MC}} + \Delta E_J$ is our estimate of the minimum energy per particle from all possible Jastrow trial functions. ΔE_3 is our estimate of the energy shift introduced by three-body factors in the ground state, giving the final column $E = E_J + \Delta E_3$.

ρ (\AA^{-3})	$E_{\text{OPT}}^{\text{HNC}}$ ($^\circ\text{K}$)	E_0^{HNC}	ΔE_J	E_0^{MC}	E_J	ΔE_3	E
0.017 96	-5.223	-5.109	-0.114	-5.856	-5.970	-0.345	-6.315
0.019 46	-5.119	-4.978	-0.141	-5.958	-6.099	-0.444	-6.543
0.020 96	-4.858	-4.681	-0.177	-5.825	-6.002	-0.565	-6.567
0.021 85	-4.618	-4.414	-0.204	-5.703	-5.907	-0.656	-6.563
0.023 88	-3.846	-3.568	-0.278	-5.25	-5.53	-0.879	-6.41
0.025 71	-2.789	-2.453	-0.336	-4.73	-5.07	-1.138	-6.21
0.028 44	-0.5434	-0.102	-0.441	-3.55	-3.99	-1.630	-5.62

ground-state wave function when only two- and three-body factors are included. The method of approach used here—considering first the Jastrow function (i.e., two-body factors) and then adding three-body factors—is sensible if the energy converges rapidly as higher-order factors are included. We are encouraged by the fact that the contribution of the three-body factors is less than 10% of either the potential or kinetic energy obtained from the Jastrow function, and can hope that the contribution of four-body factors would be down by another order of magnitude, contributing of the order of 0.1°K per particle to the binding energy. We have no proof of that though and a calculation is not presently feasible.

Assuming that two- and three-body factors in the trial ground-state wave function are adequate for the task of determining the binding energy and structure function for the ground state, we still found it necessary to make further approximations in the variational calculation. The approximation in the Jastrow calculation of Sec. IV was the HNC approximation, which we then attempted to correct by the reference procedure employing the Monte Carlo calculation for the parametrized Jastrow function. An equivalent approximation is to say that

the shift in the Jastrow energy obtained by the paired-phonon analysis ΔE_J of Tables VII and IX would be the same in an exact calculation as it is in the HNC calculation. We expect the error in that assumption to be a few percent of ΔE_J , meaning that the uncertainty in the binding energy due to this approximation is probably less than 0.05°K .

The error in the final step of our calculation—the inclusion of three-body factors (Sec. V)—is much more difficult to assess. There are two approximations in that calculation. The first is the use of the convolution approximation for the three-body structure function. The convolution approximation does not satisfy a self-consistency condition for the three-body optimization procedure like that satisfied by the HNC approximation in Sec. III. Consequently the three-body optimization cannot be iterated. Thus the second approximation is the use of Eq. (73) to obtain the three-body contributions to energy rather than calculating the energy directly from an extended Jastrow function after several iterations.

The accumulation of uncertainty is difficult to estimate precisely, but a conservative guess is that the calculated binding energy is in error by as much as 0.5°K . Thus we are not yet able to choose

TABLE IX. Energy terms for the ground-state energy per particle of ${}^4\text{He}$ interacting by the MDD-2 potential of Eq. (64). The notation is identical to Table IV.

ρ (\AA^{-3})	$E_{\text{OPT}}^{\text{HNC}}$ ($^\circ\text{K}$)	E_0^{HNC}	ΔE_J	E_0^{MC}	E_J	ΔE_3	E
0.017 96	-4.933	-4.692	-0.241	-5.672	-5.913	-0.467	-6.380
0.019 46	-4.654	-4.360	-0.294	-5.621	-5.915	-0.609	-6.524
0.020 96	-4.160	-3.811	-0.349	-5.325	-5.674	-0.785	-6.459
0.021 85	-3.763	-3.360	-0.403	-5.059	-5.462	-0.905	-6.367
0.023 88	-2.548	-2.004	-0.544	-4.31	-4.85	-1.226	-6.080
0.025 71	-1.017	-0.345	-0.672	-3.50	-4.17	-1.581	-5.753

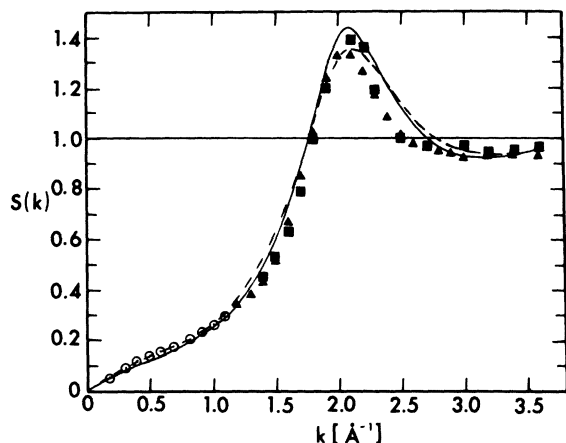


FIG. 6. Liquid-structure function of liquid ${}^4\text{He}$ at $\rho_0 = 0.02185 \text{ \AA}^{-3}$ calculated from the extended Jastrow trial function including three-body factors [Eq. (65)]. The dashed line uses the Lennard-Jones potential and the solid line uses the MDD-2 potential. The experimental points are labeled as in Fig. 2.

the best of the two potential energies discussed here. We have hopes of removing the HNC approximation for ΔE , in the not too distant future by performing a Monte Carlo calculation of the paired-phonon analysis function $\mathcal{K}(k)$. Improving the three-body calculation requires a new approximation for the three-body distribution function satisfying a self-consistency condition, or a Monte Carlo calculation of the three-body version of $\mathcal{K}(k)$. The latter is prohibitively expensive, but a direct calculation of the total energy including three-body factors determined by some approximation may be possible.³⁴

We conclude by noting that the results of this calculation using the Lennard-Jones potential have been applied elsewhere to the calculation of the density dependence of the roton parameters in liquid ${}^4\text{He}$.³⁵ We found a substantial improvement over previous calculations when compared to experiment with most of the improvement due to the three-body factors.³⁵ Indeed the agreement there is much better than that shown in Fig. 5(a) for the peak in $S(k)$, which is closely related to the roton parameters. The difference may be due to the fact that the roton parameters are measured at lower temperature (1.3 °K) than the finite-pressure structure function of Fig. 5(a).

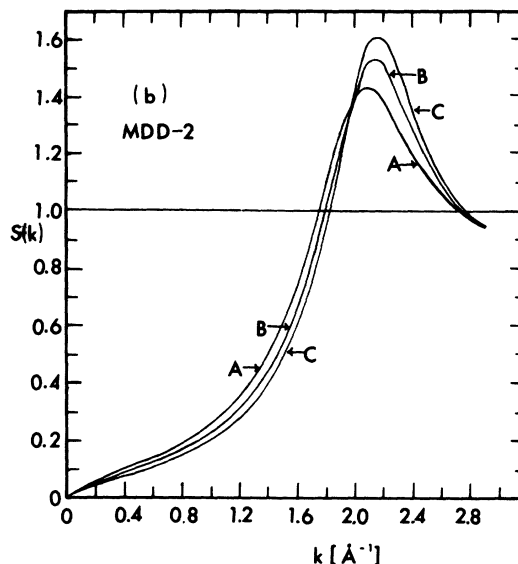
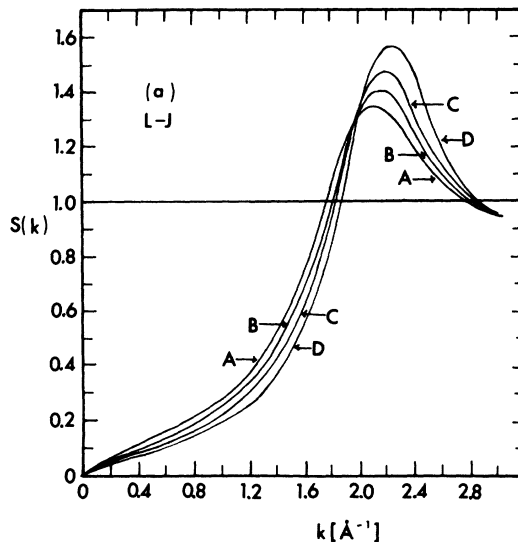


FIG. 7. Liquid-structure function at several densities calculated from the extended Jastrow function including three-body factors [Eq. (65)]. (a) Lennard-Jones potential is used; (b) the MDD-2 potential is used. The densities are A, 0.02185 \AA^{-3} ; B, 0.02388 \AA^{-3} ; C, 0.02571 \AA^{-3} ; and D, 0.02844 \AA^{-3} .

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We would like to acknowledge a helpful discussion about helium interaction potentials with R. D. Murphy.

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