# Effect of Explicit Three-Particle Correlations on the Liquid Structure Function of Helium 4†

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The discrepancies that exist between theory and experiment in the ground-state energy and the liquid structure function of $He^4$ are not insignificant. We show via a two-dimensional Monte Carlo calculation that by incorporating explicit three-particle correlation factors into the variational wave function, both the energy and the liquid structure function are improved in the right direction. This suggests that the discrepancies need not be attributed to the choice of the potential.

The ground-state energy $E_0$ and the liquid structure function $S(k)$ of liquid $He^4$ have been measured with high accuracy. $E_0$ is known to be $-7.14°K/N$, and $S(k)$, defined through the radial distribution function $g(r)$ by

$$S(k) = 1 + \rho\int[g(r) - 1]e^{i\vec{k}\cdot\vec{r}}d^3r, \quad (1)$$

is given in Fig. 1. On the latter, the neutron scattering data of Cowley and Woods[1] and the x-ray scattering data of Achter and Meyer[2] and Hallock[3] show reasonably good agreement with one another.

Over the last decade, a number of variational calculations have been carried out[4] for the ground state of liquid $He^4$, all of which made use of the Jastrow function

$$\psi_J(1, 2, \cdots, N) = \prod_{i<j} \exp[\tfrac{1}{2}u(r_{ij})] \quad (2)$$

and the Lennard-Jones 6-12 potential with parameters determined by deBoer and Michels. The form of $u(r)$ varied a great deal; also the many-body integration techniques differed much in approach as well as in practice. The numerical results obtained were, however, nearly identical. $E_0$ stands at $E_J \approx -6°K/N$, and $S(k)$ or $g(r)$ shows much less structure than experimental data. For comparison, see Fig. 1.

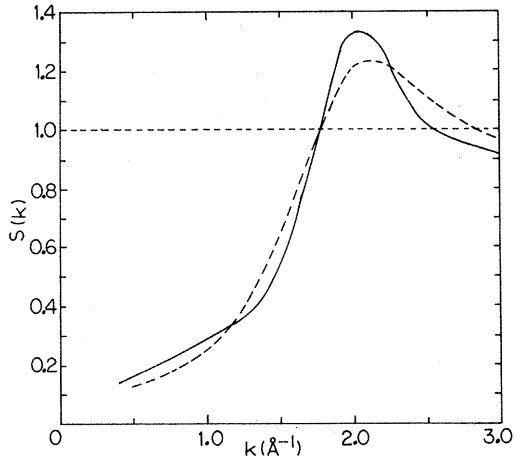


FIG. 1. Liquid structure function $S(K)$ for bulk $He^4$. Solid curve, experiment; dashed curve, Jastrow theory.

There are two sources to which we can attribute the discrepancies. One concerns the accuracy of the deBoer-Michels potential. The other concerns the variational wave function. Surely the energy will be lowered and the liquid structure sharpened if the potential is made more attractive by, e.g., deepening the potential well. Recent work in the literature indeed reflects continued concern and interest in redetermining the potential.[5] However, one must still have faith in the quantum mechanical calculation that follows. It is unreasonable to modify the potential in order to force an inaccurate calculation artificially into agreement with experiment. For this reason, we prefer to concentrate first on improving the variational calculation.

The Jastrow function explicitly takes into account only two-particle correlations. For the system to lower its energy, every triplet should tend to form an equilateral triangle, so as to allow themselves to sample more of one another's attraction. This calls for explicit three-particle correlations not contained in Jastrow functions. We therefore take a new trial wave function of the form

$$\psi(1, 2, \cdots, N) = \prod_{i<j} \exp[\tfrac{1}{2}u(r_{ij})] \times \prod_{k<l<m} \exp[\tfrac{1}{2}w(r_{kl}, r_{lm}, r_{mk})] \quad (3)$$

and vary $w(r_{kl}, r_{lm}, r_{mk})$ to minimize the expectation value

$$E = \langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle, \quad (4)$$

where

$$H = \sum_i \frac{-\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} v(r_{ij}). \quad (5)$$

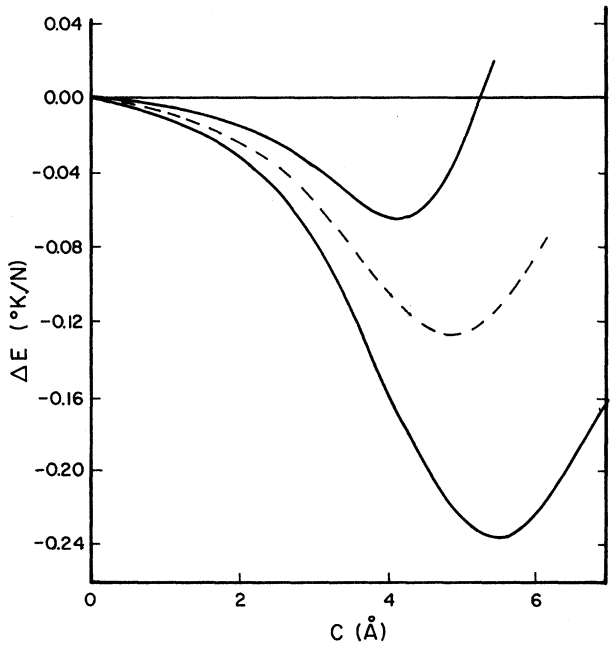


FIG. 2. Improvement in energy $\Delta E$ as a function of the variational parameter $C$ for two independent runs along with the average.

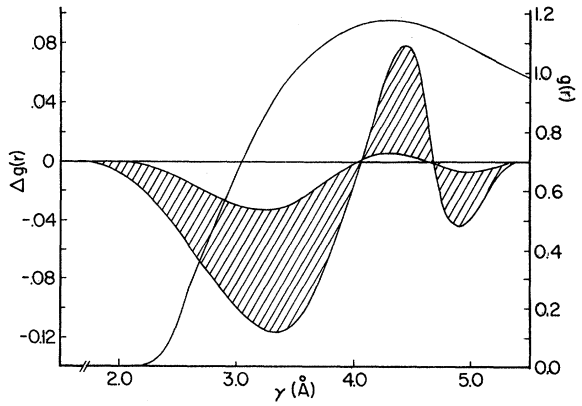


FIG. 3. Improvement in the pair distribution function, $\Delta g(r)$. The spread indicated on $\Delta g(r)$ represents both the uncertainty in the minimum value for $C$ and low statistics; however, while the magnitude of $\Delta g(r)$ changes with $C$ the locations of the peaks and valleys do not. The Jastrow $g(r)$ is also shown.

The evaluation of $E$ was carried out using a biased-selection Monte Carlo integration technique to be described elsewhere.[6] To save computer time, the calculation was done in two dimensions in the belief that an extrapolation of our conclusions to three dimensions is meaningful. First a Jastrow calculation was carried out using a popular form of the wave function:

$$u(r) = -(b/r)^5. \tag{6}$$

The energy minimum occured at $b = 2.94$ Å. The results were checked against earlier work performed by one of us in collaboration with Miller and Campbell[7] using a variety of integral equation techniques. Having satisfied ourselves that the Monte Carlo method could reproduce, and indeed improve upon, earlier results,[6] we introduced three-particle factors in the convenient form[8]

$$w(r, s, |\vec{r} - \vec{s}|) = -(C/R)^n \equiv w(R), \tag{7}$$

where

$$R^2 = r^2 + s^2 + |\vec{r} - \vec{s}|^2. \tag{8}$$

The choice of $w$ was based on the fact that, for positive $n$, equilateral triangles are favored over a large class of other less-structured configurations. Instead of evaluating $g(r)$ and

$$\frac{E}{N} = \frac{\sigma}{2}\int g(r)\left\{v(r) - \frac{\hbar^2}{4m}\left[u''(r) + \frac{u'(r)}{r}\right]\right\} d^2r + \frac{\sigma^2}{6}\int g_3(r, s, |\vec{r} - \vec{s}|)\left\{\frac{3\hbar^2}{8m}\left[w''(R) + \frac{3w'(R)}{R}\right]\right\} d^2r\, d^2s \tag{9}$$

(where $\sigma$ is the areal density taken at the equilibrium value 0.0358 Å$^{-2}$ and $g_3$ is the three-particle distribution function) directly, we calculated the change $\Delta g(r)$ in $g(r)$ due to the inclusion of three-particle factors, the $g_3$, and the change in energy $\Delta E \equiv E - E_J$, using the same configurations as in the Jastrow calculation. This can be done with the biased-selection Monte Carlo method since the system is not simulated but rather the integrals are evaluated over a set of statistically independent configurations. Each configuration contained 25 particles with periodic boundary conditions. This would correspond to 125 particles in three dimensions. Numerically varying the parameter $C$ for various values of $n$, we estimated that the energy minimum was at $C \approx 4.4$ Å for $n = 4$. The minimum value of $\Delta E$, shown in Fig. 2, amounts to $(-0.12 \pm 0.06)$°K/$N$, which is about 18% of the two-dimensional $E_J$ of $(-0.68 \pm 0.08)$°K/$N$. $\Delta g(r)$ is given in Fig. 3, and the corresponding improvement in the liquid structure function $\Delta S(k)$ is given in Table I along with $S(k)$ from the Jastrow calculation. By inspecting Table I, it is

TABLE I. Improvement in the two-dimensional liquid structure function. Column 3 corresponds to the upper bound of the curve in Fig. 3 and column 4 corresponds to the lower bound.

| $k(\text{Å}^{-1})$ | Jastrow S(k) | S(k) | |
|---|---|---|---|
| 0.5 | 0.749 | -0.043 | -0.011 |
| 0.7 | 0.796 | -0.012 | -0.002 |
| 0.9 | 0.888 | 0.014 | 0.006 |
| 1.1 | 1.024 | 0.029 | 0.009 |
| 1.3 | 1.159 | 0.032 | 0.008 |
| 1.5 | 1.225 | 0.025 | 0.005 |
| 1.7 | 1.194 | 0.010 | 0.001 |
| 1.9 | 1.098 | -0.007 | -0.003 |
| 2.1 | 0.999 | -0.021 | -0.005 |
| 2.3 | 0.934 | -0.025 | -0.005 |
| 2.5 | 0.907 | -0.017 | -0.003 |
| 2.7 | 0.906 | -0.001 | 0.000 |
| 2.9 | 0.920 | 0.013 | 0.002 |
| 3.1 | 0.948 | 0.019 | 0.003 |
| 3.3 | 0.981 | 0.012 | 0.003 |
| 3.5 | 1.011 | 0.000 | 0.001 |
| 3.7 | 1.031 | -0.010 | -0.001 |
| 3.9 | 1.042 | -0.012 | -0.002 |
| 4.1 | 1.046 | -0.005 | -0.002 |
| 4.3 | 1.041 | 0.004 | -0.001 |

clear that the improvements are all in the right directions, even though the magnitude of $\Delta S(k)$ is small throughout. These preliminary results suggest to us that an improved variational wave function which contains explicit three-particle correlation factors is capable of producing results in good agreement with experiment without modifying the potential. To lend certainty to this remark, one must improve the statistics, enlarge the wave-function space, and carry out an exhaustive search for the optimum three-particle function. Also one must extend these calculations to three dimensions. We regret that computer time requirements cause us to postpone such investigations.

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[1]R. A. Cowley and A. D. B. Woods, Can. J. Phys. 49, 177 (1971).

[2]E. K. Achter and L. Meyer, Phys. Rev. 188, 291 (1969).

[3]R. B. Hallock, Phys. Rev. A 5, 320 (1972).

[4]See, for example, E. Feenberg, *Theory of Quantum Fluids* (Academic, New York, 1969), Chap. 6.

[5]L. W. Bruch and I. J. McGee, J. Chem. Phys. 46, 2959 (1967), and 52, 5884 (1970). In this work we take the Lennard-Jones 6-12 potential with $\epsilon = 10.22°K$ and $\sigma = 2.556$Å as determined by deBoer and Michels.

[6]R. L. Coldwell, Phys. Rev. A (to be published), and to be published.

[7]M. D. Miller, C.-W. Woo, and C. E. Campbell, Phys. Rev. A (to be published).

[8]A new form suggested by one of us [C.-W. Woo, Phys. Rev. Lett. 28, 1442 (1972)] was not yet available at the time of this work.