MOMENTUM DISTRIBUTIONS

Edited by

Richard N. Silver
Los Alamos National Laboratory
Los Alamos, New Mexico

and

Paul E. Sokol
The Pennsylvania State University
University Park, Pennsylvania

Plenum Press • New York and London

MOMENTUM DISTRIBUTION IN LIQUID ^{4}HE AT LOW TEMPERATURES: VARIATIONAL METHODS

Efstratios Manousakis

Department of Physics and
Center for Materials Research and Technology
Florida State University, Tallahassee, Florida 32306

ABSTRACT

We review variational calculations of the momentum distribution and condensate fraction of atoms in liquid ^4He at zero and low temperatures. We use ground state and excited state wave functions which include Jastrow, three-body and backflow correlations and are obtained from variational calculations that give accurate energies and pair distribution functions over a wide density range. We calculate the change of the ground state momentum distribution due to creation of an elementary excitation and use it to calculate the change of the momentum distribution and condensate fraction at low temperatures ($T < 1°K$). This calculation brings out the collective and single-particle character of the excitations in the long and short wavelength limit respectively and the interplay between the two at intermediate momenta. The expectation values are calculated by means of cluster expansions and making use of the hypernetted-chain equation and the scaling approximation to include the contribution of the elementary diagrams. We discuss the singularities of the momentum distribution at low momenta and low temperatures. We compare our results with momentum distributions obtained from Green's function Monte Carlo calculations and neutron scattering data.

1. INTRODUCTION

A great deal of theoretical effort has been invested towards a microscopic understanding of the ground state of dense quantum fluids in terms of the bare interaction between the constituent particles. Liquid helium is unique for it remains liquid even at absolute zero where the quantum coherence has fundamental consequences and for the simplicity of the atom-atom interaction. Five decades ago, London[1] proposed that the underlying mechanism, which drives the superfluid transition in the isotope liquid ^4He, is the Bose-Einstein condensation. It was already sixties when, after the suggestion of Miller, Pines and Nozières[2] that the condensate could be probed by neutron scattering experiments, Hohenberg and Platzman[3] proposed a definite deep inelastic neutron scattering experiment. The neutrons at high momentum transfers

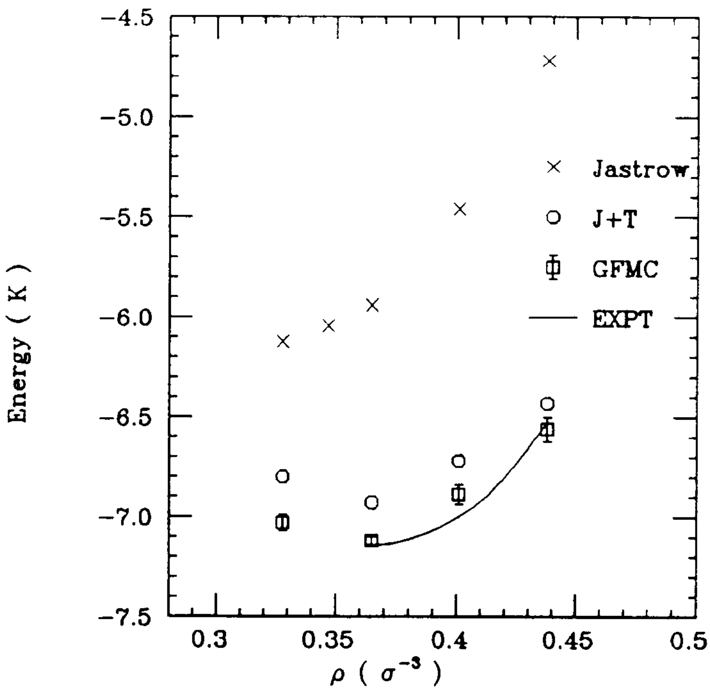

Figure 1. The ground state energy for several densities calculated with Jastrow (crosses), Jastrow plus triplets (open circles) is compared with the GFMC (open squares) results and experiment (solid line).

interaction and they are very close to the experimental curve (solid line). The crosses represent the results obtained with the Jastrow wave-function (1.1).

The open circles obtained with the $J + T$ wave function are within 4% of the GFMC energies. The same wave function gives ground state energies for droplets of liquid ^4He which are also within $\sim 4\%$ of the presumably exact GFMC energies. The structure function obtained with the $J + T$ wave function is in excellent agreement with the GFMC results and experiment. We conclude that the Aziz potential and the approximate wave function (1.2) give good quantitative description of the ground state of liquid ^4He.

The nontrivial task in the variational calculations is the accurate evaluation of the expectation values with the wave functions (1.1) and (1.2). In Ref. 7 and 8 the Hypernetted-Chain-Scaling (HNC/S) approximation was introduced where scaling techniques were employed to include the contribution of the elementary diagrams. The results obtained with this technique are within < 1% agreement with the Monte Carlo integration techniques.

Wave functions and energies of elementary excitations in liquid ^4He have been studied by many authors. The first variational wave function of an elementary excitation with momentum $\vec{k}$ was the Bijl-Feynman ansatz

$$\psi_{\vec{k}} = \sum_{i=1}^{N} e^{i\vec{k}.\vec{r}_i}\psi_0. \tag{1.5}$$

Namely

$$n_{\bar{x}}(\vec{p}) = \int \rho_{\bar{x}}(\vec{r}_{11'}) e^{i\vec{p}.\vec{r}_{11'}} d^3 r_{11'}. \tag{2.3}$$

Using the wave function (1.2) for the ground state $n_0(p)$ is obtained as

$$n_0(p) = n_c N \delta_{p,0} + n'_0(p), \tag{2.4a}$$

$$n'_0(p) \equiv \int \Big(\rho_0(r) - \rho_0(r \to \infty)\Big) e^{i\vec{p}.\vec{r}} d^3 r \tag{2.4b}$$

where n_c is the condensate fraction and $n'_0(p)$ represents the momentum distribution at finite p. The Kronecker-δ, which represents the $p = 0$ condensate is a result of the off-diagonal long-range order in the one-body density matrix

$$\rho_0(r_{11'} \to \infty) = n_c \rho. \tag{2.5}$$

Here ρ denotes the particle density.

TABLE I

$n_0(p)$ at the equilibrium density $\rho = 0.365\sigma^{-3}$.

p	$n_0(p)$	p	$n_0(p)$
0.015	5.01	0.65	0.38
0.035	2.36	0.85	0.29
0.050	1.81	1.05	0.22
0.055	1.66	1.25	0.15
0.075	1.33	1.45	0.10
0.095	1.14	1.65	0.058
0.115	1.02	1.85	0.033
0.135	0.93	2.05	0.024
0.155	0.86	2.25	0.020
0.175	0.81	2.45	0.015
0.195	0.76	2.65	0.009
0.215	0.73	2.85	0.006
0.235	0.70	3.05	0.003
0.250	0.69	3.25	0.002
0.450	0.50	3.35	0.001

The one-particle density matrix has been calculated in Ref. 14 using the $J + T$ wave function. Both n_c and $\rho_0(r_{11'})$ are functions of the usual and auxiliary distribution and nodal functions as well as elementary diagrams which are summed using the HNC/S technique. The accuracy of this approximation in calculating $\rho_0(r_{11'})$ was demonstrated[14] in the simpler case of Jastrow wave functions where excellent agreement was found with existing results of MC integration. Here, skipping the technical details of the calculation, we review some of the main results with the realistic $J + T$ wave function.

It may be verified that the asymptotic behavior (1.3) reflects the following singularity in $n_0(p)$

$$n_0(p \to 0) = n_c \frac{mc}{2\hbar} \frac{1}{p}\,. \tag{2.6}$$

which is half of the total phonon energy obtained with both the Bijl-Feynman and Feynman-Cohen wave functions in the $k \to 0$ limit. Thus, a phonon in Bose liquids is, indeed, a pure harmonic vibration with half of its energy from kinetic and the other half from potential terms.

In the short-wavelength limit ($k \to \infty$)

$$t_0(k \to \infty) = t_+(k \to \infty) = 1 \tag{3.5a}$$

$$t_-(k \to \infty) = t'(k \to \infty) = 0. \tag{3.5b}$$

i.e, a single particle is removed from the ground state distribution and is put in the distribution $n_0(|\vec{p} - \vec{k}|)$ centered at $\vec{p} = \vec{k}$. In this limit the energy of the Feynman excitation is $\hbar^2 k^2/2m$ and equals the change in the kinetic energy.

In Fig. 2a, we give $t_0(k)$, $t_+(k)$ and $t_-(k)$ as calculated for finite k using Eq. (1.6) and (1.2) for $\psi_{\vec{k}}$ and ψ_0 respectively and in the HNC/S approximation.

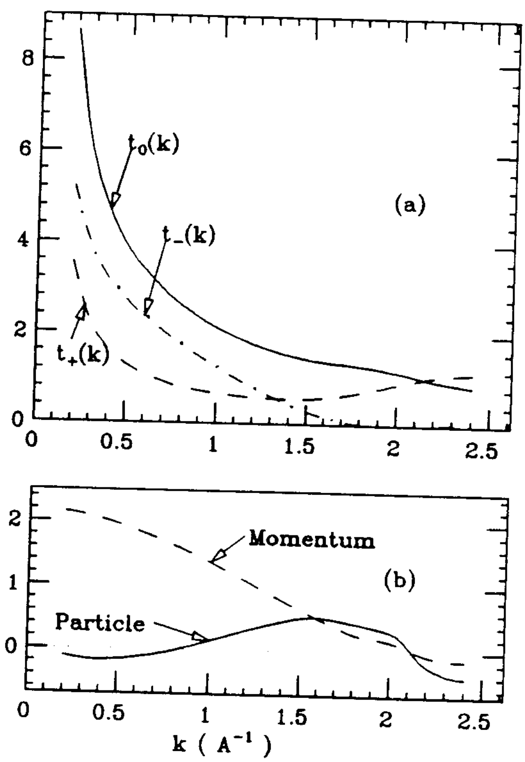

Figure 2. (a) The functions $t_0(k)$, $t_+(k)$ and $t_-(k)$. (b) The contributions $t'_n(k)$ and $t'_m(k)$ of the t' term to the particle and momentum conservations. k is the momentum of the excitation.

If we neglect the term t' for a moment, the creation of a single elementary excitation of momentum $\vec{k}$ removes $t_0(k)$ particles from the ground state momentum distribution;

In this temperature range ($T < 1^\circ K$) only long-wavelength phonons can be excited, i.e excitations with $k < 0.2\mathring{A}^{-1}$. In Ref. 12 and 13, we found that the wave function (1.6) is accurate for such excitations i.e with energies $e(k < 0.2\mathring{A}^{-1}) < 4^\circ K$. In this temperature range, we may neglect the δn_3 term because the integral of t' is small for $k < 0.2\mathring{A}^{-1}$. In this range of k and T, we can further approximate $e(k \to 0) = \hbar ck$ and $t_0(k)$, $t_+(k)$ and $t_-(k)$ by the expressions (3.3). Therefore, we obtain

$$\delta n_1(T,p) \simeq -\frac{m}{12\hbar^3\rho c}T^2 n_0(p) = -\left(\frac{T}{T_0}\right)^2 n_0(p), \tag{4.3a}$$

$$\delta n_2(T,p) = \int \frac{d^3k}{(2\pi)^3\rho}\frac{1}{\exp(\beta e(k)) - 1}\frac{mc}{\hbar c}n_0(\vec{p} - \vec{k}), \tag{4.3b}$$

$$n(T,p) = \left(1 - \left(\frac{T}{T_0}\right)^2\right)n_0(p) + \delta n_2(T,p). \tag{4.3c}$$

where $T_0 \sim 7.6K$. Thus, the temperature dependence of the condensate fraction at low T is given by

$$n_c(T) = n_c(0)\left(1 - \left(\frac{T}{T_0}\right)^2\right). \tag{4.4}$$

The last equation has also been derived by a phenomenological approach[16] and from the structure of perturbation theory at finite T[17].

The term $Nn_c\delta_{p,0}$ in $n_0(p)$ gives rise to terms in δn_2 which have singular behavior in the $p \to 0$ limit. These singular terms are

$$\delta n_s(T,p) = \frac{n_c(0)mc}{\hbar p}\frac{1}{\exp(\beta e(k)) - 1} \simeq \frac{n_c(0)m}{\hbar^2\beta}\frac{1}{p^2} - \frac{n_c(0)mc}{2\hbar}\frac{1}{p} + \ldots \tag{4.5}$$

$n_0(p)$ has exactly the same $1/p$ singularity with opposite sign (see Eq. (2.6)). Thus, for $\beta\hbar cp << 1$, the $1/p$ term in $n_0(p)$ is canceled by that in $\delta n(T,p)$. This cancelation has also been pointed out by Griffin[18]. The present method can provide $\delta n(T,p)$ for small T but for any p. In Ref. 15 we give tables of the change $\delta n(T,p)$ for several values of T and p obtained with the full $\delta n_{\vec{k}}(\vec{p})$. It appears that the expression

$$n(T,p) \simeq \left(1 - \left(\frac{T}{T_0}\right)^2\right)n_0(p) + \frac{n_c(0)mc}{\hbar p}\frac{1}{\exp(\beta\hbar ck) - 1} \tag{4.6}$$

is a good approximation for low T and it may be used in neutron scattering experiments to find the contribution from the singular terms. The $\delta n(T, p \neq 0)$ is positive in this temperature range; thus, it appears that the atoms are removed from the $p = 0$ condensate and placed in states with $\hbar cp \lesssim \pi T$.

5. RESULTS AND COMPARISONS

In Fig. 3 we compare the results of our calculations of the momentum distribution at the equilibrium density with the GFMC[19] and the neutron scattering data[20]. The solid line is our $n_0(p \neq 0)$ obtained with the wave function (1.2) which includes optimized Jastrow and three-body correlations. In these results the $n(p)$ is normalized such that

$$\int n(p)d^3p = 1. \tag{5.1}$$

The dashed-dotted curve is the result of the GFMC calculation obtained from a simulation of 64 particles in a periodic box. The differences at low p and the small differences at intermediate and higher p between the variational $n_0(p)$ and that obtained by the GFMC calculation may be attributed either a) to the approximate nature of the

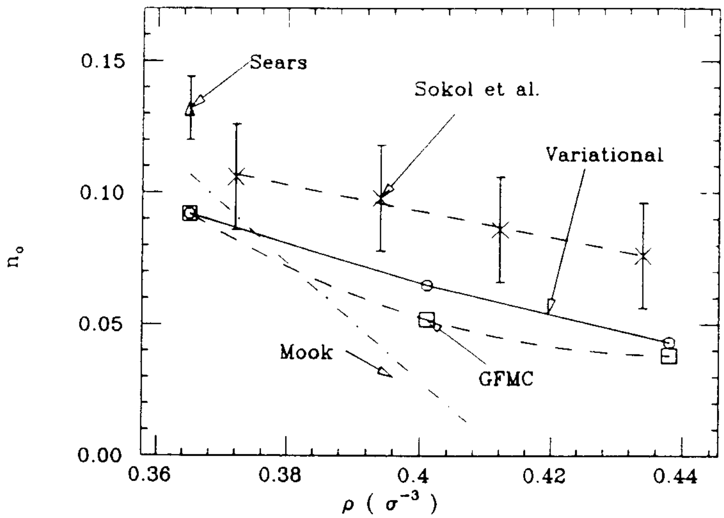

Figure 4. The condensate fraction as a function of density as obtained from the variational calculation (solid line) compared with GFMC and experimental results. The lines are guides to the eye.

At $T < 1°K$, the condensate fraction depends weakly on temperature. Using Eq.(4.4) and taking $n_c(0) = 0.092$ we find $n_c(T = 1°K) = 0.090$, which is a negligible difference.

6. ACKNOWLEDGEMENTS

This work was supported in part by the Florida State University Supercomputer Computations Research Institute which is partially funded by U.S Department of Energy through contract No DE-FC05-85ER250000.

REFERENCES

1. F. London, Nature (London) **141**, 643 (1938); Phys. Rev. **54**, 947 (1938).
2. A. Miller, D. Pines, and P. Nozières, Phys. Rev. **127**, 1452(1962).
3. P. C. Hohenberg and P. M. Platzman, Phys. Rev. **152**, 198(1966).
4. M. H. Kalos, M. A. Lee, P.A. Whitlock and G. V. Chester, Phys. Rev. **B 24**, 115 (1981).
5. R. A. Aziz, V. P. S. Nain, J. S. Carley, W. L. Taylor and D. T. Mcconvill, J. Chem. Phys. **70**, 4330 (1979).
6. K. Schmidt, M. H. Kalos, M.A. Lee and G. V. Chester, Phys. Rev. Lett. **45**, 573 (1980).
7. Q. N. Usmani, B. Friedman and V. R. Pandharipande, Phys. Rev. **B 25**, 6123(1983).
8. Q. N. Usmani, S. Fantoni, and V. R. Pandharipande, Phys. Rev. **B 26**, 6123(1983).
9. L. Reatto and G. V. Chester, Phys. Lett. **22**, 276(1966).
10. R. P. Feynman and M. Cohen, Phys. Rev. **102**, 1189(1956).
11. V. R. Pandharipande, Phys. Rev. **B 18**, 218(1978).
12. E. Manousakis and V. R. Pandharipande, Phys. Rev. **B 30**, 5062(1984).
13. E. Manousakis and V. R. Pandharipande, Phys. Rev. **B 33**, 150(1986).