Momentum Distribution of Liquid $^4$He Across the Normal–Superfluid Phase Transition

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Abstract We have carried out a study of the momentum distribution and of the spectrum of elementary excitations of liquid $^4$He across the normal–superfluid transition temperature, using the path integral Monte Carlo method. Our results for the momentum distribution in the superfluid regime show that a kink is present in the range of momenta corresponding to the roton excitation. This effect disappears when crossing the transition temperature to the normal fluid, in a behavior currently unexplained by theory.

Keywords Superfluid helium · Momentum distribution · Quantum Monte Carlo

1 Introduction

Continued theoretical and experimental work in the last decades has led to an accurate knowledge of the superfluid transition in liquid $^4$He [1]. Probably, the most important feature is the suppression of the superfluid density above the critical temperature $T_\lambda = 2.17$ K. The condensate fraction, which quantifies the macroscopic occupation of the zero-momentum state, vanishes at the same point. The nature of the excitations of the system is also modified in a significant way. By means of neutron scattering, one can have access to the dynamic structure function $S(k, \omega)$ which contains the maximum attainable information on the excitations of the fluid [2]. In fact, the richness of $S(k, \omega)$ in superfluid $^4$He has been emphasized in recent and highly accurate experiments.
The most noticeable feature in the dynamic response when \( T \) is crossed is the disappearance of the roton as a quasiparticle mode and, as a consequence, of the conditions for superfluidity according to the Landau criterion. The behavior of the momentum distribution of the \( ^4 \)He atoms is notably different in the two sides of the transition, the change being mainly in the limit of low momenta. First of all, in the superfluid regime, the presence of a condensate gives rise to a sharp delta contribution at \( k = 0 \). Furthermore, \( n(k) \) shows a singular \( \frac{1}{k} \) behavior which can be explained in terms of a coupling between the condensate and the long-wavelength excitations (phonons) \([4,5]\). On the other hand, the width of the roton mode increases slightly with \( T \) by a purely thermal effect. However, some theoretical calculations in the limit of zero temperature point out that the shape of \( n(k) \) presents a change in the slope of a kink at \( k \approx 0.1 \) \text{Å}^{-1} \( -1 \). This effect is due to the evolution of the roton energy and condensation density with temperature that is described by the form:

\[
(\langle f^\dagger f - n_f \rangle) = \sum_{\omega_n} \frac{Z}{\omega_n - \omega} \phi^2 = \sum_{\omega_n} \frac{Z}{\omega_n - \omega} \phi^2 = \frac{1}{N} \sum_{\omega_n} \frac{Z}{\omega_n - \omega} \phi^2 = A + Y = H
\]  

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The aim of this paper is to investigate the relation between the presence of the kink in \( n(k) \) and that of the roton mode in \( S(k, \omega) \). For this purpose, we perform path integral Monte Carlo (PIMC) simulations of \(^4\)He across the normal–superfluid transition and we calculate both the momentum distribution and the roton energy and strength. Our results show that as the liquid enters the normal phase, the kink in \( n(k) \) and that of the roton mode in \( S(k, \omega) \) can be related to the presence of the roton, thus supporting the hypothesis that the kink in the momentum distribution is a signal of the presence of the roton.

2 The Path Integral Monte Carlo Method

At the microscopic level, liquid \(^4\)He can be described as a quantum \( N \)-body system, whose Hamiltonian takes the form:

\[
\hat{H} = \hat{K} + \hat{V} = -\frac{\hbar^2}{2m} \nabla^2 + \sum_{i<j} V(|\mathbf{r}_i - \mathbf{r}_j|),
\]  

where \( m \) is the mass of a \(^4\)He atom. The interaction between two particles in \( \mathbf{r} \) and \( \mathbf{r}' \) is accurately described by the Aziz potential \([10]\). The properties of this system at a finite temperature \( T \) are obtained from the thermal density matrix \( \hat{\rho} \), where \( Z \) is the partition function and \( \beta = 1/(k_B T) \).
constant, and \( Z = \text{Tr}(e^{-\beta \hat{H}}) \) is the partition function. The knowledge of \( \hat{\rho} \) allows for the calculation of the expected value of any operator \( \hat{O} \),

\[
\langle \hat{O} \rangle = \text{Tr}(\hat{\rho} \hat{O}) = \int d\mathbf{R} \ \rho(\mathbf{R}, \mathbf{R}; \beta) O(\mathbf{R}),
\]

where in the last term of the equation we have used the coordinate representation, \( \mathbf{R} = \{r_1, \ldots, r_N\} \) being the set of coordinates of the \( N \) particles in the system. Deep in the quantum regime, i.e., at very low temperature, the estimation of the thermal density matrix is unfeasible, due to the non-commutativity of the kinetic and potential energy operators appearing in the Hamiltonian (Eq. 1). Nevertheless, this problem can be overcome applying the convolution property of \( \hat{\rho} \) and rewriting Eq. 2 as

\[
\langle \hat{O} \rangle = \int d\mathbf{R}_1 \ldots d\mathbf{R}_M \prod_{j=1}^{M} \rho(\mathbf{R}_j, \mathbf{R}_{j+1}; \tau) O(\mathbf{R}_1 \ldots \mathbf{R}_M),
\]

with \( M \) being an integer and \( \tau = \beta/M \). In this way, the thermal density matrix at the desired temperature \( T \) is obtained from a product of density matrices at a higher temperature \( MT \), where the effects of the non-commutativity of \( \hat{K} \) and \( \hat{V} \) are reduced and it is easy to build approximations for the quantum density matrix.

For a Bose system, the function \( \rho(\mathbf{R}_j, \mathbf{R}_{j+1}; \tau) \) is positive definite and the product appearing in Eq. 3 can be considered as a probability distribution. Thus, the thermal averages \( \langle \hat{O} \rangle \) can be efficiently estimated with a stochastic Monte Carlo technique, the so-called path integral Monte Carlo (PIMC) method [11]. Although increasing the number \( M \) of convolution terms (usually called beads) in Eq. 3 allows to reduce the systematic error due to the approximation of the thermal density matrix and eventually to recover “exactly” the expectation values, it is fundamental to use a good approximation for the thermal density matrix in order to reduce the numerical complexity of the algorithm and to avoid ergodicity issues in the sampling. To this end, we use a fourth-order time-step (\( \tau \)) approximation [12], based on a symplectic expansion of the propagator due to Chin [13],

\[
e^{-\tau \hat{H}} = e^{-v_1 \tau \hat{W}_{a_1}} e^{-t_1 \tau \hat{K}} e^{-v_2 \tau \hat{W}_{l-2a_1}} e^{-t_1 \tau \hat{K}} e^{-v_1 \tau \hat{W}_{a_1}} e^{-2\tau \hat{K}},
\]

where \( \hat{W}_{a_1} = \hat{V} + \frac{u_0}{v_1} a_1 \tau^2 [\hat{\nabla}, \hat{\nabla}], \hat{\nabla} \) with \( \hat{K} \) and \( \hat{V} \) being the kinetic and potential operators, respectively. A set of parameters \( t_0, t_1, v_1, v_2, a_1, u_0 \) must be optimized in order to achieve a good convergence of the propagator.

An additional difficulty in the PIMC simulations of liquid \( ^4\text{He} \) at low temperatures arises from the indistinguishability of the particles. This problem can be solved sampling numerically the bosonic permutations among the atoms: We have used the worm algorithm which is an efficient method aimed at this goal [14].

The PIMC method is able to give an accurate description of the static properties of Bose systems, but it does not allow for the calculations of real-time correlation functions, which are fundamental to study dynamic properties, such as the spectrum of the elementary excitations. A quantity that is easily accessible in PIMC simulation is the intermediate scattering function \( F(k, \tau) = 1/N \langle \hat{\rho}_k(\tau) \hat{\rho}^\dagger_k(0) \rangle \), with \( \hat{\rho}_k(\tau) = \hat{\rho}(\mathbf{R}, \mathbf{R}; \beta) e^{-i \mathbf{k} \cdot \mathbf{R}} \)
\[ \sum_{i=1}^{N} e^{-i k \cdot r_i} \] being the density fluctuation operator. This function \( F(k, \tau) \) can be considered as a correlation function in imaginary time and it can be related to the dynamic structure factor \( S(k, \omega) \) by a Laplace transform. Even if the inversion of the Laplace transform is an ill-posed problem, many numerical algorithms have been developed to recover reasonable estimates of \( S(k, \omega) \) from the PIMC data for \( F(k, \tau) \) [15–19]. In this work, to obtain the dynamic structure factor, we use a stochastic optimization algorithm based on simulated annealing, as described in Ref. [20].

### 3 Results

We have performed PIMC calculations of liquid \(^4\)He following the SVP (saturated vapor pressure) and \( \rho = 10.13 \) bar densities, from \( T = 0.8 \) to \( 4 \)K, with \( N = 64 \) particles in the simulation box under periodic boundary conditions. We have checked that the use of larger number of particles does not modify the main results discussed in this section.

Following Eq. 3, we implemented the calculation of the one-body density matrix, defined as

\[
\rho_1(r_1, r'_1) = \frac{V}{Z} \int d r_2 \ldots d r_M \rho(R, R'; \beta),
\]

where \( \rho(R, R'; \beta) \) is the thermal density matrix computed for two configurations \( R = \{r_1, r_2, \ldots, r_N\} \) and \( R' = \{r'_1, r_2, \ldots, r_N\} \) which differs for the position of only one particle. We reported the influence of the temperature on this function in Fig. 1, sampled from non-diagonal configurations along the simulation.

As it is well known, there are significant differences between results for \( \rho_1(r) \) obtained below and above the critical temperature \( T_\lambda \). In the superfluid regime, \( T < T_\lambda \), the one-body density matrix shows a plateau at large distances corresponding to the presence of a finite occupation of the zero-momentum state. Instead, in the normal phase, \( T > T_\lambda \), the one-body density matrix decays exponentially to zero pointing to the absence of off-diagonal long-range order in the system.

The momentum distribution \( n(k) \) can be obtained from the Fourier transform of the one-body density matrix \( \rho_1(r) \) (Eq. 5) as

\[
n(k) = n_0 \delta(k) + \rho \int d^3 r e^{i k \cdot r} (\rho_1(r) - n_0),
\]

where \( \rho \) stands for the density of our system and \( n_0 = \lim_{r \to \infty} \rho_1(r) \) is the condensate fraction. Results of \( n(k) \) for a range of temperatures across \( T_\lambda \) are reported in Fig. 2, plotted as \( kn(k) \). Our data start at a \( k \) value compatible with the finite size of the system, \( k_{\text{min}} = 2\pi / L \), with \( L \) the length of any side of the cubic simulation box. Therefore, we are not able to show the \( k \to 0 \) behavior of the momentum distribution.

When \( T \) increases, we see a progressive broadening of the distribution due to a classical thermal effect. However, in this evolution with \( T \) we can observe a non-trivial effect that appears at intermediate \( k \) values, \( 1.5 < k < 2.5 \text{ Å}^{-1} \). As we show in Fig. 2, and in particular in the inset, there is a kink of \( n(k) \) within this \( k \) range for temperatures
smaller than $T_\lambda$, i.e., in the superfluid regime. As the temperature increases, and goes near the transition point, the kink becomes smoother, and it completely disappears for $T > T_\lambda$. We also notice that the kink is a bit more pronounced at SVP, when the intensity of the roton peak in the dynamic structure factor is larger (see Fig 3a). The location of this kink around $k \simeq 2 \text{Å}^{-1}$ leads us to think that the kink can be related to the characteristic momentum of the roton excitation. It is known that the roton quasiparticle excitation is associated with the superfluidity of the system through the Landau criterium. In the normal phase, the roton disappears as a quasiparticle peak in the dynamic response $S(k, \omega)$. Therefore, the connection between this kink in $n(k)$ and the roton excitation seems rather plausible.

The evolution of the roton with temperature has been studied by means of the inverse Laplace transform of the intermediate scattering function [20], as commented in the previous section. In Fig. 3 (left panel), we show how the maximum height of the dynamic structure factor slowly decreases in the superfluid phase as we increase the temperature, until it experiences an abrupt drop once we enter the normal phase and then it remains constant. This is an expected result since the quasiparticle peak of the roton excitation disappears once we cross $T_\lambda$. Our data, reported in the figure, also show that the strength of the roton peak is slightly reduced when the pressure increases.

We can also look for the energy of the roton excitation, as well as the phonon and maxon excitations, and see how they evolve with temperature (see Fig. 3, right panel).
In the superfluid phase, for the roton, the energy decreases as we increase the temperature. At higher temperatures, in the normal phase, it seems that the energy raises again, but one cannot really speak about roton mode anymore due to the substantial broadening of its peak. As a matter of comparison, we report in Fig. 3 data obtained for the maxon and phonon energies. For the maxon excitation, the behavior is similar to the one of the roton, but in this case the strength of the peak when crossing $T_\lambda$ is not so drastically reduced [20]. In the case of the phonon, the influence of the temperature is much smaller than in the previous cases.
Fig. 3 Top Maximum height of the dynamic structure factor $S(k, \omega)$ of the roton ($k \sim 1.91 \text{ Å}^{-1}$) across the normal–superfluid phase transition. All data are normalized by the maximum height at $T = 0.8$ K and SVP. Bottom Temperature dependence of the phonon ($k \sim 0.43 \text{ Å}^{-1}$), maxon ($k \sim 1.24 \text{ Å}^{-1}$) and roton ($k \sim 1.91 \text{ Å}^{-1}$) energy. Experimental results for the roton energy from Ref. [21]. In both figures $k_R$ and $\omega_R$ are the momentum and the energy of the roton, respectively (Color figure online)

4 Conclusions

We have carried out a microscopic study of the momentum distribution of liquid $^4$He at finite temperature using the PIMC method. Our aim has been to determine the possible origin of the kink that $n(k)$ shows at $k$ values around the roton momentum. This is not the first observation of this kink in theoretical calculations since it was already obtained more that twenty years ago [6]. The location of the kink around the roton
momentum led the idea of its relation with the roton but without further analysis. Now, we have shown that this scenario is more plausible because the kink vanishes when $T_\lambda$ is crossed, mimicking the behavior of the roton quasiparticle peak.

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