Microscopic calculation of the phonon-roton branch in superfluid $^4$He

J. Boronat and J. Casulleras

Departament de Física i Enginyeria Nuclear, Campus Nord B4-B5,
Universitat Politècnica de Catalunya, E-08028 Barcelona, Spain

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Abstract

Diffusion Monte Carlo results for the phonon-roton excitation branch in bulk liquid $^4$He at zero temperature are presented. The sign problem associated to the excited wave function has been dealt both with the fixed-node approximation and the released-node technique. The upper bounds provided by the fixed-node approximation are shown to become exact when using the released-node method. An excellent agreement with experimental data is achieved both at the equilibrium and near the freezing densities.

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The physical nature of the excitations in superfluid $^4$He at low momenta is still nowadays not completely well understood [1], in contrast with the vast knowledge of its static properties. In a pioneering work, Landau [2] proposed a model for the elementary excitations to explain the superfluidity of liquid $^4$He. From a different point of view, Bogoliubov [3] calculated the excitation spectrum of a weakly interacting Bose gas where the condensate fraction, i.e., the fraction of particles in the zero momentum state, plays an explicit role. Both theories predict a continuous dispersion curve which starts with a phonon excitation, reaches a first maximum (maxon), lowers to a local minimum (roton), and then grows up as the energy of a free particle. From general ideas on the nature of the excitations in an interacting Bose fluid, Feynman [4] proposed the first microscopic approach to the problem. The Feynman trial wave function provides a qualitative description of the excitation spectrum but fails in reproducing the roton energy by a factor two. Later on, Feynman and Cohen [5] included backflow correlations in the trial wave function, reducing in one half the differences between the experimental data and the original Feynman’s prediction. Following Feynman’s language, the phonon-roton branch corresponds to collective density-like excitations where the condensate fraction does not enter in an explicit way. Recently, it has been argued by Glyde and Griffin [6] that the continuous spectrum results from the superposition of density excitations, dominating in the phonon region, and single-particle excitations, important in the roton minimum. This theory has emerged after the experimental determination of the temperature dependence of the excitation spectrum which shows the phonon peak in the dynamic structure function $S(q, \omega)$ at both sides of the $\lambda$-transition whereas the roton practically disappears in the normal phase.

In the last years a considerable effort has been made to improve quantitatively the microscopic predictions for the phonon-roton excitation spectrum $\varepsilon(q)$. Manousakis and Pandharipande [7] calculated $\varepsilon(q)$ by means of the correlated basis function (CBF) method using a basis of Feynman-Cohen states. The variational Monte Carlo (VMC) method using shadow wave functions has also proved to be quantitatively quite efficient in the calculation of $\varepsilon(q)$ [8] in spite of its approximate description of the ground state. The application of $ab$
\textit{initio} Monte Carlo methods to this problem has been, however, severely hindered by the sign problem associated to the excited wave function. Only recently, Boninsegni and Ceperley \cite{9} have calculated $\varepsilon(q)$ by means of a path integral Monte Carlo (PIMC) calculation of $S(q,\omega)$ from a Laplace inversion of the imaginary-time correlation factor $S(q,t)$. However, for noisy data this inversion is an ill-posed problem that prevents a model-independent determination.

In the present work, we present a zero temperature calculation of the phonon-roton spectrum using the diffusion Monte Carlo (DMC) method. In this method, the imaginary-time Schrödinger equation for the function $f(R,t) = \psi_T(R)\Phi(R,t)$,

$$-rac{\partial f(R,t)}{\partial t} = -D\nabla^2_R f(R,t) + D\nabla_R (F(R)f(R,t)) + (E_L(R) - E)f(R,t), \quad (1)$$

is solved stochastically, $\Phi(R,t)$ and $\psi_T(R)$ being the wave function of the system and a trial wave function used for importance sampling, respectively. In the above equation, $E_L(R) = \psi_T^{-1}(R)H\psi_T(R)$ is the local energy and $F(R) = 2\psi_T^{-1}(R)\nabla_R \psi_T(R)$ acts as a quantum drift force; $D = \hbar^2/2m$, with $m$ the mass of the particles, and $R$ stands for the $3N$-coordinate vector of the $N$ particles. In the asymptotic regime, $f(R,t \rightarrow \infty) \rightarrow \psi_T(R)\Phi(R)$ where $\Phi(R)$ corresponds to the lowest energy eigenstate of the system not orthogonal to the trial wave function $\psi_T(R)$. For a thorough description of the DMC method see, for instance, Refs. \cite{10,11}.

The wave function $\psi(R)$ corresponding to a phonon-roton excitation is an eigenstate of the momentum operator. As pointed out by Feynman \cite{4}, this requirement is achieved with the simple model wave function

$$\psi^F(R) = \sum_{i=1}^{N} e^{iq \cdot r_i} \psi^0(R), \quad (2)$$

$\psi^0(R)$ being the ground-state wave function. The first correction to $\psi^F(R)$, originally proposed by Feynman and Cohen \cite{5}, includes backflow correlations. In this case, the excited wave function is given by

$$\psi^{BF}(R) = \sum_{i=1}^{N} e^{iq \cdot \tilde{r}_i} \psi^0(R), \quad (3)$$
where

$$\tilde{r}_i = r_i + \sum_{j \neq i} \eta(r_{ij}) r_{ij}.$$  \hspace{1cm} (4)

The inclusion of backflow correlations improves appreciably the variational results of $\varepsilon(q)$ with respect to the Feynman’s choice but the quantitative agreement with experiment is still poor, specially near the roton minimum.

In the DMC implementation a real probability distribution function $f(R, t)$ is suitable. Therefore, we choose as importance sampling wave function $\psi_T(R)$ the superposition of two excitations of momenta $q$ and $-q$ which are degenerate in energy:

$$\psi_{TF}^F(R) = \sum_{i=1}^{N} \cos(q \cdot r_i) \psi_0^0(R)$$  \hspace{1cm} (5)

at Feynman’s level, and

$$\psi_{BF}^{RF}(R) = \sum_{i=1}^{N} \cos(q \cdot \tilde{r}_i) \psi_T^0(R) \hspace{1cm} (6)$$

when backflow correlations are included.

In a first step, the sign problem associated to the excited wave function has been dealt within the framework of the fixed-node (FN) approximation \[10\]. The FN approximation provides an upper bound to the exact value and has been extensively used in the study of fermionic systems. In what concerns the calculation of excited states, we have recently used the FN-DMC method to study a vortex excitation in two-dimensional superfluid $^4$He \[12\]. Within FN, the sign problem is avoided by imposing the nodal surface of the trial wave function to the excited Monte Carlo wave function. The problem is hence mapped onto a bosonic calculation with a well defined density probability function. Beyond this approximation, one can remove the nodal constraint of the FN approach using a released-node technique (RN) \[13\]. This method makes use of an auxiliary guiding function $\psi_g(R)$, positively defined everywhere. Random walkers are then allowed to cross the nodal surface (becoming negative) and to survive for a finite lifetime $t_r$. The RN approach provides the exact eigenvalue in the limit of large surviving times, but presents the disadvantage...
of becoming numerically unstable in the limit \( t_r \to \infty \) where the number of positive and negative walkers become similar.

The success of the method, i.e., the achievement of an asymptotic regime before the growth of the statistical errors, is closely related to the quality of \( \psi_T(R) \) and \( \psi_g(R) \). The guiding function \( \psi_g(R) \) has to approach \( |\psi_T(R)| \) away from the nodal surface and must be non-zero in the nodes to make possible the flux of walkers through it. We have taken the simple model

\[
\psi_g(R) = \left( \psi_T(R)^2 + a^2 \right)^{1/2},
\]

which satisfies both requirements for a proper choice of the value of the parameter \( a \). In fact, the value given to the parameter \( a \), which has to be of the same order of magnitude than the mean value of \( |\psi_T(R)| \), governs the flux of walkers through the nodes. Therefore, the relaxation time of the release process is a function of \( a \): when the value of \( a \) is increased the relaxation time is reduced and vice versa.

The released-node energy is obtained projecting out the excited state modeled by \( \psi_T(R) \). This projection is carried out assigning to each walker a weight \( W(R) \) given by

\[
W(R) = \sigma(R) \frac{|\psi_T(R)|}{\psi_g(R)},
\]

\( \sigma(R) \) being +1 (−1) for an even (odd) number of crossings. The released-node energy is thus determined through

\[
E_{RN}(t_r) = \frac{\sum_{t \leq t_r} W(R) E^T_L(R)}{\sum_{t \leq t_r} W(R)},
\]

where the sums are extended to all the surviving walkers with a lifetime less than \( t_r \), and \( E^T_L(R) = \psi_T(R)^{-1} H \psi_T(R) \).

In our computation we have considered a simulation box with 108 \(^4\)He atoms interacting through the HFD-B(HE) Aziz potential \([2]\), and at two densities, \( \rho_0 = 0.365 \sigma^{-3} \) and \( \rho_P = 0.438 \sigma^{-3} \) (\( \sigma = 2.556 \) \( \text{Å} \)). The density \( \rho_0 \) corresponds to the equilibrium density, and \( \rho_P \) is close to the freezing density. The ground-state correlations have been modeled by a two-body wave function originally proposed by Reatto \([3]\),
\[ \psi^0_T(R) = \prod_{i<j} \exp \left\{ -\frac{1}{2} \left( \frac{b}{r_{ij}} \right)^5 - \frac{L}{2} \exp \left[ -\left( \frac{r_{ij} - \lambda}{\Lambda} \right)^2 \right] \right\} , \] (10)

which we have previously employed in ground-state calculations [11]. The function \( \eta(r) \), entering in the backflow wave function (4), has been chosen to be a gaussian

\[ \eta(r) = A \exp \left[ -\left( \frac{r - r_b}{\omega_b} \right)^2 \right] \] (11)
as in the variational calculation of Ref. [7]. The values of the parameters in Eqs. (10,11) are \( b = 1.20 \sigma, L = 0.2, \Lambda = 0.6 \sigma, \lambda = 2.0 \sigma, A = 0.15, r_b = 0.8 \sigma, \) and \( \omega_b = 0.44 \sigma, \) which are roughly the optimal ones at the equilibrium density \( \rho_0 \). The parameter \( a \) appearing in the guiding wave function \( \psi_g(R) \) has been taken as \( a = 3.0 \) for all the \( q \) values, and the largest lifetime \( t_r \) used corresponds to 190 DMC sweeps. The same set of parameters have been used at the highest density \( \rho_P \).

As mentioned before, the released-node energy estimation would be exact in the limit of large lifetimes. However, the computational effort to simultaneously enlarge \( t_r \) and maintain the statistical fluctuations into an acceptable level grows with \( t_r \). Having estimated a reasonable upper limit of \( t_r \), given the present computational resources, we can study the influence of the excited trial wave function in the RN energy. As a general trend, if the RN energy does not reach a constant regime within \( t_r \), an improved model for the excited trial wave function should be used. The empirical way in which we have studied the asymptotic regime of the RN energy is by fitting the function

\[ E(t_r) = E_\infty + C e^{-t_r/\tau} \] (12)
to the largest \( t_r \) values. In the interpretation of the MC results, we have followed the guideline of accepting only the RN values that do not present discrepancies between the largest \( t_r \) data and the asymptotic limit \( E_\infty \). The fit (12) has been used to decide whether to trust or not the MC values but not to provide the asymptotic limit.

We have verified that at \( \rho_0 \), and for values \( q < 2.5 \text{ Å}^{-1} \), the RN energies using the Feynman wave function (5) do reach the expected constant regime, the difference between
the largest $t_r$ calculated energy and the value of $E_\infty$ predicted by the $\chi^2$-fit ([12]) being less than the statistical error. This is not the case for $\rho_P$. At this high density, that agreement only subsists for the lowest $q$ value and for the value of $q$ nearest to the roton. For the other values of $q$ we have had to include backflow correlations ([8]) to reach the asymptotic limit. This fact is illustrated in Fig. 1, where the excitation energy

$$\varepsilon(q) = \frac{\langle \psi_T(q) | H | \Phi(q) \rangle}{\langle \psi_T(q) | \Phi(q) \rangle} - \frac{\langle \psi_0^T | H | \Phi_0 \rangle}{\langle \psi_0^T | \Phi_0 \rangle}$$

(13)

per particle is plotted as a function of $t_r$ for $q = 1.11$ Å$^{-1}$ and $q = 1.84$ Å$^{-1}$. Near the roton, $q = 1.84$ Å$^{-1}$, both the Feynman and backflow results show a coincident asymptotic value without a significant slope. At $q = 1.11$ Å$^{-1}$, near the maxon energy, the situation is clearly different: the backflow results have reached a constant behaviour whereas the Feynman ones show a slow approach to the correct value, which has not been achieved yet for the maximum value of $t_r$. The latter behaviour is also observed for the highest value of $q$ ($q \simeq 2.6$ Å$^{-1}$) both at $\rho_0$ and $\rho_P$. In this case, the inclusion of backflow correlations in the wave function is not enough to eliminate the bias and a significant difference exists between the largest $t_r$ energy and the asymptotic value predicted by the numerical fit ([12]).

The released-node mechanism suppresses the fixed-node constraints and drives the calculation to the exact excitation energy, as shown in Table I. In the table, fixed-node values using $\psi_T^F$ and $\psi_F^{BF}$, and the released-node estimation are compared with experimental data ([16]) at the equilibrium density $\rho_0$. The FN results with backflow correlations improve the Feynman ones for the three values of $q$ in a magnitude which depends on $q$. Thus, the inclusion of backflow correlations seems slightly more relevant in the roton than in the maxon. On the other hand, the RN excitation energies agree with the experimental data for the three values of $q$ within the statistical errors.

In Fig. 2 the RN excitation energies are compared with the experimental spectrum ([16]) at $\rho_0$. The RN results correspond, for each $q$, to the last point in the release process, the error bars being only the statistical errors. As commented before, the systematic errors are less than the statistical ones except for the highest $q$ result ($q = 2.58$ Å$^{-1}$). For this
latter value of $q$ we also report an estimation coming from the extrapolation supplied by the fit \([12]\). Apart from this point, where the RN method shows the shortcomings of the backflow wave function at a so high value of $q$, the agreement between the RN results and the experiment is excellent. As a matter of comparison, the FN results using $\psi_r^{BF}$ are also plotted. It is worth noticing the difference between the FN energies in the maxon and in the roton regimes; the roton is reproduced quite accurately whereas in the maxon the backflow correlations overestimate appreciably the excitation energies. At the highest $q$, where the spectrum bends down, the FN energy is quite far from the experimental data.

As is well known from neutron scattering data, the location and depth of the roton minimum depends on the density. Thus, when the density increases the roton appears shifted to higher momenta and its energy decreases. The energies in the maxon region increase with the density but in an amount not so well experimentally known as in the roton. In Fig. 3, we report the RN excitation energies at $\rho_P$ in comparison with experimental data \([17]\). There is, again, a good agreement between theory and experiment within the statistical errors except at the highest $q$ evaluated ($q = 2.74 \, \text{Å}^{-1}$) where the RN energy has not reached a constant value inside the release interval.

In conclusion, we have shown that the diffusion Monte Carlo method in conjunction with the fixed-node technique, and more specially, with the released-node method provides a very useful tool to study excitations in correlated quantum many body systems like liquid $^4$He. The results for $\epsilon(q)$ are in an excellent quantitative agreement with experimental data, both at the equilibrium and near the freezing densities, improving previous variational and CBF results and providing an exact description of one of the oldest and hardest problems in the study of quantum fluids from a microscopical viewpoint. Possible applications of the RN-DMC method would be the ripplon excitations in a free liquid $^4$He surface or the determination of the excitation energy of a single impurity in bulk liquid $^4$He. On the other hand, the interpretation of the roton excitation as a single-particle mode deserves further theoretical work from a microscopical viewpoint \([18]\).

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FIGURES

FIG. 1. Excitation energies per particle as a function of the lifetime $t_r$ at $\rho_P$. The full circles are obtained using $\psi_T^{BF}$ and the diamonds using $\psi_T^F$.

FIG. 2. Phonon-roton spectrum at the equilibrium density $\rho_0$. The full circles are the RN results and the diamonds correspond to a FN calculation with $\psi_T^{BF}$. The open square, which has been slightly shifted to the right for clarity, is the result of the extrapolation with the fit (12). The solid line is the experimental data from Ref. [16].

FIG. 3. Phonon-roton spectrum at the density $\rho_P$. Same notation as in Fig. 2. The experimental data is from Ref. [17].
TABLE I. Excitation energies at $\rho_0$ in comparison with experimental data. The FN-$\psi_T^F$ and FN-$\psi_T^{BF}$ columns are the fixed-node energies using $\psi_T^F$ and $\psi_T^{BF}$, respectively. The RN column corresponds to the released-node estimation. Experimental data is taken from Ref. [16].

| $q$ (Å$^{-1}$) | FN-$\psi_T^F$ (K) | FN-$\psi_T^{BF}$ (K) | RN (K) | Expt. (K) |
|---------------|-------------------|----------------------|--------|-----------|
| 0.369         | 7.56 ± 0.49       | 7.24 ± 0.38          | 7.02 ± 0.49 | 7.0       |
| 1.106         | 18.47 ± 0.49      | 16.52 ± 0.43         | 13.82 ± 0.43 | 13.8      |
| 1.844         | 13.82 ± 0.54      | 10.37 ± 0.59         | 9.18 ± 0.59  | 8.9       |
Figure 1

![Graph showing data points for two different wavevectors, q=1.11 Å\(^{-1}\) and q=1.84 Å\(^{-1}\). The graph plots ε/N (K) against t_r, where ε/N varies with t_r.]
Figure 2

The graph shows the relationship between $q$ (Å$^{-1}$) and $\varepsilon$ (K). The data points are represented by various markers and error bars, with a smooth curve fitting through the data. The x-axis represents $q$ (Å$^{-1}$), ranging from 0.0 to 3.0, while the y-axis represents $\varepsilon$ (K), ranging from 0 to 30.
Figure 3

\[ \varepsilon (\text{K}) \] vs. \[ q (\text{Å}^{-1}) \]