Bounds for the phonon-roton dispersion
in superfluid $^4$He

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(February 28, 1995)

Abstract

The sum rule approach is used to derive upper bounds for the dispersion law
$\omega_0(q)$ of the elementary excitations of a Bose superfluid. Bounds are explicitly
calculated for the phonon-roton dispersion in superfluid $^4$He, both at equilib-
rium ($\rho = 0.02186$ Å$^{-3}$) and close to freezing ($\rho = 0.02622$ Å$^{-3}$). The bound
$\omega_0(q) \leq 2S(q) |\chi(q)|^{-1}$, where $S(q)$ and $\chi(q)$ are the static structure factor
and density response respectively, is calculated microscopically for several val-
ues of the wavevector $q$. The results provide a significant improvement with
respect to the Feynman approximation $\omega_F(q) = q^2(2mS(q))^{-1}$. A further,
stronger bound, requiring the additional knowledge of the current correlation
function is also investigated. New results for the current correlation function
are presented.

67.40.-w, 67.40.Db
I. INTRODUCTION

The microscopic investigation of the dynamic behavior of superfluid $^4$He has been the object of extensive theoretical work in the past starting from the pioneering works by Bijl and Feynman [1] (see, for instance, Ref. [2] for an up-to-date review). Recent approaches, based on perturbation theory with correlated functions [3] and on the use of shadow variables [4], have provided accurate predictions for the dispersion law of this strongly interacting Bose system.

The purpose of this paper is to show that in a Bose superfluid the knowledge of relevant static properties of the system can be used to derive useful upper bounds for the excitation spectrum, employing a sum rule approach (for a recent discussion on sum rules in Bose superfluids see for example Ref. [5]). We will show that a key role in this context is played by the static density response for which Diffusion Monte Carlo (DMC) calculations have recently become available [6]. Another relevant quantity in this context is the kinetic structure function, for which new DMC results will be presented.

Explicit results for various bounds at the equilibrium density, $\rho = 0.02186 \text{ Å}^{-3}$, as well as close to freezing, $\rho = 0.02622 \text{ Å}^{-3}$, will be given in the first part of the work. In the second part we will discuss in detail the behaviour of the static response function, extending the analysis of Ref. [7] to lower $q$’s and high pressure.

II. BOUNDS FOR THE PHONON-ROTON DISPERSION

The most famous estimate of the dispersion law in a Bose superfluid was proposed many years ago by Bijl and Feynman [1]. The resulting dispersion can be written in the form

$$\omega_F(q) = \frac{m_1(q)}{m_0(q)} = \frac{q^2}{2mS(q)},$$

where

$$m_k(q) = \int_0^\infty d\omega \, \omega^k S(q, \omega)$$
are the $k$th-moments of the dynamic structure function $S(q, \omega)$ ($\hbar = 1$ in this work). In deriving Eq. (1) one has evaluated the moment $m_1$ through the well known f-sum rule [8]

$$m_1(q) = \frac{1}{2} \left\langle [\rho_{-q}, [H, \rho_q]] \right\rangle = N \frac{q^2}{2m}$$

(3)

holding for systems of particles interacting with velocity independent potentials. The brackets $\langle \ldots \rangle$ denote ground state averages, while $H$ is the $N$–body Hamiltonian of the system

$$H = -\sum_{i=1}^{N} \nabla_i^2 \frac{2m}{2} + \sum_{i<j}^{N} V(r_{ij}) ,$$

(4)

and $\rho_q$ is the density fluctuation operator

$$\rho_q = \sum_{i=1}^{N} e^{-i qr_i} .$$

(5)

The moment $m_0$ has been instead expressed in terms of the static structure factor $S(q)$ through the equation

$$m_0(q) = \langle \rho_{-q} \rho_q \rangle = NS(q) .$$

(6)

Both results (3) and (6) have been obtained using the completeness relation. The static structure factor $S(q)$ is known with great accuracy both from Monte Carlo calculations and experimental data. In the present work we use the Diffusion Monte Carlo results shown in Fig. 1.

The Feynman energy (1), being based on the ratio of the two moments $m_1$ and $m_0$, provides, at zero temperature, a rigorous upper bound to the energy $\omega_0(q)$ of the lowest state excited by the density operator $\rho_k$,

$$\omega_0(q) \leq \omega_F(q) .$$

(7)

In the following we will identify the energy $\omega_0(q)$ with the one of the elementary excitations of the system, i.e., the phonon-roton spectrum (in a Bose superfluid this identification is exact apart from decay processes of the elementary mode into two or more excitations [9]).

The bound (1) reproduces exactly the phonon dispersion at small $q$:
\[ \omega_0(q) = cq \]  \hspace{1cm} (8)

where \(c\) is the sound velocity. This follows from the low \(q\) behavior of the static structure factor

\[ S(q)_{q \to 0} = \frac{q}{2mc} \]  \hspace{1cm} (9)

and is the consequence of the fact that in the macroscopic regime both the moments \(m_0\) and \(m_1\) are exhausted by the phonon mode.

At higher wave vectors the Feynman bound instead overestimates significantly the experimental dispersion law (see Fig. 2). This is due to the occurrence of multipair excitations, whose strength distribution, at energy higher than \(\omega_0(q)\), turns out to be particularly important in the determination of the energy weighted moment. For example the experimental data of Ref. [11] at s.v.p. indicate that the roton exhausts only 1/3 of the energy weighted sum rule, the remaining part being associated with high energy multipair excitations.

The idea to go beyond the Feynman approximation employing a sum rule approach was first developed many years ago by Feenberg [12] with the help of the moments \(m_2\) and \(m_3\). Here we show that better bounds can be calculated using the inverse energy weighted moment

\[ m_{-1}(q) = \int dq \omega S(q, \omega) \frac{1}{\omega} \]  \hspace{1cm} (10)

This moment is an ideal quantity in order to investigate the collective properties of a Bose superfluid. In fact the factor \(1/\omega\) quenches significantly the high frequency tail of \(S(q, \omega)\) where multipair excitations are important. Furthermore the absence of single particle excitations in the low energy part of the spectrum, typical feature of a Bose system, makes the integral (10) particularly sensitive to the contribution of the collective mode. For the same reason the experimental determination of \(m_{-1}\), through a direct integration of the dynamic structure factor measured by neutron scattering, turns out to be more accurate than the one of any other moment [11].
The inverse energy weighted sum rule (10) is directly related to the static density response of the system through the equation
\[
\chi(q) = -2m_{-1}(q) \tag{11}
\]
The static response fixes the linear changes in the density induced by an external static field interacting with the system with a potential of the form \(H_{\text{ext}} = \lambda \rho_q\), coupled to the density fluctuation operator \(\rho_q\). At small \(q\) it yields the compressibility of the system
\[
\chi(0) = -\frac{N}{mc^2} \tag{12}
\]
while at larger \(q\) is characterized by the occurrence of a pronounced peak (see discussion in Sect. II). The static response \(\chi(q)\) has been recently calculated in superfluid \(^4\)He using Diffusion Monte Carlo techniques [6]. These calculations reproduce the experimental data of \(\chi\) at s.v.p. with good accuracy.

The knowledge of the static response, together with the one of the static structure factor can be used to calculate a new upper bound for the dispersion law using the ratio
\[
\omega_{0-1}(q) = \frac{m_0(q)}{m_{-1}(q)} = \frac{2S(q)}{|\chi(q)|} \tag{13}
\]
between the non energy weighted and the inverse energy weighted sum rules. Since at zero temperature \(S(q, \omega) = 0\) for \(\omega < 0\), the following inequality rigorously holds:
\[
\omega_0(q) \leq \omega_{0-1}(q) \leq \omega_F(q) \tag{14}
\]
At small \(q\) also the bound (13) approaches the phonon dispersion law as one can immediately see using results (9) and (12). In Fig. 2 the new bound is reported for several values of \(q\). The improvement with respect to the Feynman bound is significant both in the roton and in the maxon region. As already anticipated this improvement is the consequence of the fact that the moments \(m_0\) and \(m_{-1}\), entering Eq. (13), are much less affected by multipair excitations with respect to the moment \(m_1\). This is also true at high pressure, as shown in Fig. 3.
A further improvement of the bound \((13)\) can be obtained with the help of the energy weighted moments \(m_1\) and \(m_2\). In fact one can derive the following inequality for the excitation energy \(\omega_0(q)\):

\[
\omega_0(q) \leq \frac{1}{2} \left[ \omega_{0-1} - \bar{\epsilon} - \sqrt{(\omega_{0-1} - \bar{\epsilon})^2 + 4\omega_{0-1}\Delta} \right]
\]  \(15\)

This bound is stronger than the bound \((14)\). It involves the knowledge of the variance

\[
\Delta(q) = \frac{m_1(q)}{m_0(q)} - \frac{m_0(q)}{m_{-1}(q)}
\]  \(16\)

and of the energy

\[
\bar{\epsilon}(q) = \Delta^{-1}(q) \left[ \frac{m_2(q)}{m_0(q)} + \left( \frac{m_0(q)}{m_{-1}(q)} \right)^2 - 2\frac{m_1(q)}{m_{-1}(q)} \right].
\]  \(17\)

The latter depends not only on the moments \(m_{-1}\), \(m_0\) and \(m_1\), already discussed above, but also on the moment \(m_2\). The quantity \(\Delta\) vanishes when \(q \to 0\) since the two energies \(\omega_{0-1}(q)\) and \(\omega_F(q)\) coincide in this limit as already pointed out before. Viceversa, the energy \(\bar{\epsilon}\), which represents an average energy of multipair excitations, is expected to depend less critically on \(q\). Inequality \((15)\) can be derived by using the fact that \(S(q,\omega)\) vanishes for \(\omega\) less than \(\omega_0(q)\) in bulk liquid \(^4\)He; thus the following inequality holds for any positive \(\gamma\):

\[
\omega_0 \leq \frac{\int d\omega S(q,\omega)(1 + \gamma\omega)^2}{\int d\omega S(q,\omega)\omega^{-1}(1 + \gamma\omega)^2}.
\]  \(18\)

The same inequality can be written in terms of the moments \(m_k\), and the value of \(\gamma\) can be chosen in such a way to minimize the right hand side. After some algebra one obtains inequality \((15)\). A similar procedure can be used to derive upper and lower bounds to the static response function (see Ref. \([7]\)), and will be employed in Sect. \([III]\).

The moment \(m_2\) was first explored by Feenberg \([12]\) and turns out to be proportional to the current correlation function. In fact one has

\[
m_2(q) = q^2 \langle J_{zq}^\dagger J_{zq}\rangle,
\]  \(19\)

where \(J_{zq}\) is the \(z\)-component of the current density operator, and \(q\) is taken in the \(z\)-direction. Using the definition of the kinetic structure function \([12]\)
\[
D(q) = \frac{(N-1)}{q^2 \langle \psi_0 | \psi_0 \rangle} \int d\mathbf{r}_1 \ldots d\mathbf{r}_N [\cos(\mathbf{q} \cdot \mathbf{r}_{12}) - 1] (\mathbf{q} \cdot \nabla_1 \psi_0)(\mathbf{q} \cdot \nabla_2 \psi_0)
\]  

(20)

the following expression for the moment \( m_2(q) \) holds:

\[
\frac{m_2(q)}{m_1(q)} = \frac{q^2}{2m} (2 - S(q)) + \frac{2}{m} D(q)
\]

(21)

The kinetic structure function and, hence, the moment \( m_2 \), has been directly calculated using a Diffusion Monte Carlo algorithm. The results are shown in Figs. 4 and 5. The structure of \( D(q) \) is almost the same at the two densities here considered; the curve under pressure is shifted upwards. This is just what one expects by looking at the large \( q \) behaviour of definition (20), which yields \( D(q) \to (2m/3) \langle E_K \rangle \), for \( q \gg 2\pi \rho^{1/3} \). Our values of the mean kinetic energy \( \langle E_K \rangle \) are 14.32(5) K and 19.57(5) K at \( \rho = 0.02186 \text{ Å}^3 \) and \( \rho = 0.02622 \text{ Å}^3 \) respectively. They give an asymptotic shift of 0.3 Å\(^{-2}\), in agreement with the data plotted in Fig. 4. The curve for \( D(q) \) at equilibrium density is also similar to the one used in Ref. [7]; in that case, the quantity \( D(q) \) was obtained by Fourier transforming the results of Path Integral Monte Carlo calculations [15] of the current correlation function in \( \mathbf{r} \)-space.

The microscopic results for the moments \( m_0 \), \( m_{-1} \) and \( m_2 \) allow one to calculate the bound (15); the results are reported in Figs. 2 and 3. All the moments entering this analysis have been calculated employing the Aziz potential HFDHE2 [16]. One notices a systematic improvement with respect to the bound (13) in the whole range of wavelength from maxons to rotons. At equilibrium density the bounds (1), (13) and (15) yield the roton minimum at about 17.5K, 11.8K and 10.8K, respectively, to be compared with the experimental value 8.6K. The error bars in the figures are due to statistical errors in the calculation of \( m_{-1} \) and \( m_2 \). As concerns the pressure dependence, we note that the roton minimum shifts slightly to higher wave vectors by increasing pressure, in agreement with the experimental trend [14]. Also the roton gap exhibits the correct trend, being smaller at \( \rho = 0.02622 \). However, the statistical error on \( m_{-1} \) prevents an accurate comparison with the experimental shift; in fact, the experimental roton gap decreases by only 1.3 K in the same range of pressure.
III. BOUNDS FOR THE STATIC RESPONSE FUNCTION

So far we have used theoretical data for the moments $m_{-1}$, $m_0$, $m_1$ and $m_2$ in order to evaluate rigorous upper bounds for the phonon-roton dispersion. Here we apply the formalism of Ref. [7] to evaluate upper and lower bounds to the moment $m_{-1}(q)$, and hence to the static response function $\chi(q)$, using $m_0$, $m_1$, $m_2$, $m_3$, as well as the experimental phonon-roton dispersion. This procedure will provide a check of consistency between the available theoretical calculations for the moments $m_k(q)$, extending the analysis of Ref. [7] to lower $q$'s and to high pressure.

One can easily derive lower bounds to $m_{-1}(q)$ starting from the inequality

$$\int_0^\infty d\omega \frac{S(q,\omega)}{\omega^2}(1 + \alpha \omega + \beta \omega^2)^2 \geq 0 \quad (22)$$

holding for any real $\alpha$ and $\beta$. The same inequality can be written as a lower bound to $m_{-1}(q)$. Minimization with respect to the parameters $\alpha$ and $\beta$ provide the bounds. In particular, by minimizing with respect to $\alpha$ with $\beta = 0$ one gets the Feynman approximation to $m_{-1}(q)$:

$$m_{-1}(q) \geq m_{-1}^F(q) = 2Nmq^{-2}S^2(q) \quad (23)$$

Minimizing with respect to both $\alpha$ and $\beta$ one gets a stronger lower bound:

$$m_{-1}(q) \geq \frac{m_{-1}^F(q)}{1 - \Delta(q)/\epsilon(q)} \quad (24)$$

where

$$\Delta(q) = \frac{m_2(q)}{m_1(q)} - \frac{m_1(q)}{m_0(q)} \quad (25)$$

and

$$\epsilon(q) = \Delta^{-1} \left[ \frac{m_3(q)}{m_1(q)} + \left( \frac{m_1(q)}{m_0(q)} \right)^2 - 2 \frac{m_2(q)}{m_0(q)} \right] \quad (26)$$

One notes that the quantities $\Delta$ and $\epsilon$ have the same form of $\tilde{\Delta}$ and $\tilde{\epsilon}$ in Eqs. (16) and (17), but with the index of the $k$-moments scaled by 1. Inequality (24) requires the knowledge
of the cubic energy weighted moment \( m_3(q) \), which can be calculated through the Puff sum rule \[17\]:

\[
m_3(q) = N \left[ \frac{q^2}{2m} + \frac{q^4}{m^2} \langle E_K \rangle + \frac{\rho}{2m^2} \int dr \ g(r)(1 - \cos(q \cdot r))(q \cdot \nabla)^2 V(r) \right]
\]

where \( V(r) \) and \( g(r) \) are the interatomic potential and the radial distribution function, respectively.

In a similar way, one can derive upper bounds \[7\]. One finds

\[
m_{-1}(q) \leq \frac{m_0(q)}{\omega_0(q)} = NS(q)\omega_0^{-1}(q),
\]

as well as a stronger upper bound:

\[
m_{-1}(q) \leq \frac{m_0(q)}{\omega_0(q)} \left[ 1 - \frac{m_0(q)}{m_1(q)} \left( \frac{m_1(q)}{m_0(q)} - \omega_0(q) \right)^2 \left( \frac{m_2(q)}{m_1(q)} - \omega_0(q) \right)^{-1} \right].
\]

The results for the above lower and upper bounds for \( m_{-1}(q) \) are shown in Figs. 6 and 7 at equilibrium density and close to freezing, respectively. To evaluate the bounds we have used the same \( m_k \) moments as in Sect. 1 and the experimental phonon-roton dispersion for \( \omega_0(q) \). Dashed lines correspond to the weakest bounds \[23\] and \[28\], while solid lines correspond to the bounds \[24\] and \[29\]. The latter account for the effect of multiphonon excitations through the inclusion of higher \( k \)-moments. This explains why the allowed area for \( m_{-1} \), i.e. between lower and upper bounds, is significantly reduced passing from dashed to solid lines. Indeed the bounds \[24\] and \[29\] represent a quite stringent test of consistency between independent calculations and measurements of \( k \)-moments of the dynamic structure function \( S(q, \omega) \). The available experimental data of \( m_{-1} \) at equilibrium \[11\] are consistent with the bounds. The same is true for the Diffusion Monte Carlo data \[3\] at equilibrium and freezing pressure. We note that the new Monte Carlo data for \( S(q) \) and \( D(q) \) provides accurate bounds even at relatively small \( q \)'s, i.e, in the maxon region 0.5 to 1.5 Å\(^{-1}\).

**IV. CONCLUSION**

In the first part of this work we have discussed new upper bounds for the excitation spectrum in superfluid \(^4\)He. The method makes use of basic *static* properties of the system:
the static structure factor, the static response and the current correlation function. These quantities are now available in microscopic *ab initio* calculations with good accuracy. In particular we have used recent Diffusion Monte Carlo data for the static response [6] and we present new results for the kinetic structure function. The upper bounds for the phonon-roton dispersion turn out to be rather close to the experimental values and can be calculated at any pressure.

In the second part we have evaluated upper and lower bounds to the static response function using a method proposed by two of us in Ref. [7]. The new data for the current correlation function allows one to extend the analysis of Ref. [7] to lower values of $q$ and to high pressure. The main result is a general consistency between the independent evaluations of the several $k$-moments involved in the analysis, and hence of the quantities $S(q)$, $D(q)$, $\chi(q)$ in a wide range of $q$. 


REFERENCES

[1] A. Bijl, Physica 7, 869 (1940); R.P. Feynman, Phys. Rev. 94, 262 (1954)

[2] A Griffin, Excitations in a Bose-condensed liquid, Cambridge Studies in Low Temperature Physics, Vol.4 (Cambridge University Press, Cambridge, England, 1993).

[3] E. Manousakis and V.R. Pandharipande, Phys. Rev. B 30, 5062 (1984); E. Manousakis and V.R. Pandharipande, Phys. Rev. B 33, 150 (1986)

[4] W. Wu, S.A. Vitiello, L. Reatto, and M.H. Kalos, Phys. Rev. Lett. 67, 1446 (1991)

[5] S. Stringari, Phys. Rev. B 46, 2974 (1992)

[6] S. Moroni, D. M. Ceperley, and G. Senatore, Phys. Rev. Lett. 69, 1837 (1992)

[7] F. Dalfovo and S. Stringari, Phys. Rev. B 46, 13991 (1992)

[8] D. Pines and P. Nozières, The Theory of Quantum Liquids (Benjamin, New York 1966), Vol.I; P. Nozières and D. Pines, The Theory of Quantum Liquids, (Addison Wesley, 1990), Vol.II.

[9] L. P. Pitaevskii, J. Low Temp. Phys. 87, 445 (1992)

[10] R.J. Donnelly, J.A. Donnelly, and R.N. Hills, J. Low Temp. Phys. 44, 471 (1981)

[11] R.A. Cowley and A.D.B. Woods, Can. J. Phys. 49, 177 (1971); A.D.B Woods and R.A. Cowley, Rep. Prog. Phys. 36, 1135 (1973)

[12] E. Feenberg, Theory of Quantum Fluids, (Academic Press, New York and London, 1969) ch.4; D.Hall and E.Feenberg, Ann. of Phys. 63, 335 (1971).

[13] E.C. Svensson, A.D.B. Woods, and P. Martel. Phys. Rev. Lett. 29, 1148 (1972)

[14] W.G. Stirling, in Excitations in Two- Dimensional and Three- Dimensional Quantum Fluids, eds. A.F.G. Wyatt and H.J. Lauter (Exeter 1990), NATO ASI Series B Vol. 257, p.25
[15] E.L. Pollock and D.M. Ceperley, Phys. Rev. B 36, 8343 (1987).

[16] R.A. Aziz, V.P.S. Nain, J.S. Carley, W.L. Taylor, and G.T. McConville, J. Chem. Phys. 70, 4330 (1979).

[17] R.D. Puff, Phys. Rev. 137, A406 (1965)
FIGURES

FIG. 1. Static structure factor $S(q)$ at equilibrium density (solid line) and at $\rho = 0.02622 \text{ Å}^{-3}$ (dashed line).

FIG. 2. Phonon-roton spectrum at the equilibrium density, $\rho = 0.02186 \text{ Å}^{-3}$. Solid line: experiments [10]; dashed line: Feynman approximation [1]; empty circles: upper bound $\omega_{0-1}$ defined in Eq. (13); solid circles: upper bound (15).

FIG. 3. Same as in Fig. 2 but at freezing pressure ($\rho = 0.02622 \text{ Å}^{-3}$). The solid line corresponds to a smooth interpolation between experimental data on the phonon dispersion [13], up to 1 Å$^{-1}$, and recent data on the roton minimum [14].

FIG. 4. Kinetic structure function $D(q)$ at equilibrium density (empty circles) and close to freezing (solid circles).

FIG. 5. Ratio $m_2(q)/m_1(q)$ at equilibrium density (empty circles) and close to freezing (solid circles).

FIG. 6. Inverse energy weighted moment $m_{-1}(q)$ at equilibrium density. Empty circles: experiments [11]; solid circles with error bars: Diffusion Monte Carlo calculations [6]; dashed lines: upper and lower bounds (28) and (23); solid lines: upper and lower bounds (29) and (24).

FIG. 7. Inverse energy weighted moment $m_{-1}(q)$ at density $\rho = 0.02622 \text{ Å}^{-3}$. Points with error bars: Diffusion Monte Carlo calculations [6]; dashed lines: upper and lower bounds (28) and (23); solid lines: upper and lower bounds (29) and (24).