COMMENTS

Dynamic Properties of a Nonsuperfluid Bose Liquid in the Random-Phase Approximation

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The dynamic structure factor $S(k,\omega)$ of a nonideal Bose liquid is calculated within the random-phase approximation and compared with neutron scattering data by Cowley and Woods for liquid helium in the temperature range $T_\lambda < T \leq 4.2°K$, with the conclusion that the model is wholly inadequate. A low-frequency pole in the generalized susceptibility discussed by Mattis and Landovitz is shown to be overdamped in $S(k,\omega)$.

In studying the poles of the dynamic structure factor $S(k,\omega)$ for He^4 above the X point, Mattis and Landovitz in an earlier Letter[1] concluded that not one but *two* modes of wave propagation comprised the normal modes of the system, and that the speed of propagation s of one of them fitted a law

$$s \propto (T - T_\lambda)^{1/2}$$

near T_λ, whereas the speed of the other was fairly insensitive to temperature.

In subsequent numerical work on the width of the resonances identified as these normal modes, we discovered that the widths were such that, in fact, only a single mode could be perceived, in contradiction to our earlier results. We then attempted to fit the parameters to the neutron data reported by Cowley and Woods[2] in the temperature range $T_\lambda < T \leq 4.2°K$. The most striking feature of these data is that the energy and lifetime of the well-defined collective mode observed at 1.1°K, and wave vectors $k \sim 0.2$ Å^{-1}, do not change appreciably on going from He II to He I. We find that the observed temperature dependence of the collective-mode energy is markedly different from that of the collective, random-phase–approximation (RPA) mode in the nonideal Bose liquid; nor does the wave-vector dependence of the observed mode agree with that calculated. Not surprisingly, the widths of the calculated mode are typically a factor of 50 smaller than observed values.

Our calculation is tantamount to an elaboration of ideas originally put forward by Pines[3] which exploit the analogy between the collective mode and plasmons in an electron gas. The mode results from the short-range, rather than the long-range, correlations in the liquid, and resembles the zero-sound mode proposed by Landau for Fermi fluids. Pursuing this analogy within RPA leads to an expression for the generalized sus-

ceptibility $\chi(k,\omega)$ of the form

$$\chi(k,\omega)=\chi_0(k,\omega)/[1-u\chi_0(k,\omega)] \quad (1)$$

and then[4]

$$S(k,\omega)=(2\pi nV)^{-1}\int_{-\infty}^{\infty}dt\exp(-i\omega t)\langle n_{\vec{k}}^{*}(0)n_{\vec{k}}(t)\rangle$$
$$=[\pi n\{\exp(-\beta\omega)-1\}]^{-1}\mathrm{Im}\chi(k,\omega), \quad (2)$$

where $n_{\vec{k}}$ is the particle density operator, V the volume, n the particle density, and $\beta=1/k_BT$. In (1), χ_0 represents in general more than the ideal Bose-liquid susceptibility, being that part which remains once all processes described by the polarization potential u are taken into account. For the present it suffices to know only its large-ω behavior,[5] $\chi_0(k,\omega)\to nk^2/m^*\omega^2$. If we set $\omega=sk$, then $\chi(k,\omega)$ given by Eq. (1) has a high-frequency pole at a velocity $s=(nu/m^*)^{1/2}$ which is interpreted as the observed collective mode.

Pines's discussion was taken one stage further by Etters,[6] who used the ideal Bose-liquid susceptibility to express the first-order temperature dependence of s in terms of the average kinetic energy of the individual atoms. In this instance the calculated velocity increases steadily with temperature, whereas Cowley and Woods found that the velocity corresponding to the peaks in the neutron data decreased with temperature for $T>3$°K; some of their data are shown in Fig. 1. They also found a weak dependence of this velocity on the wave vector. The question then remained as to whether a (self-consistent) RPA calculation for the nonideal Bose liquid, at finite wave vectors, would describe the data, and our conclusion is that it does not.

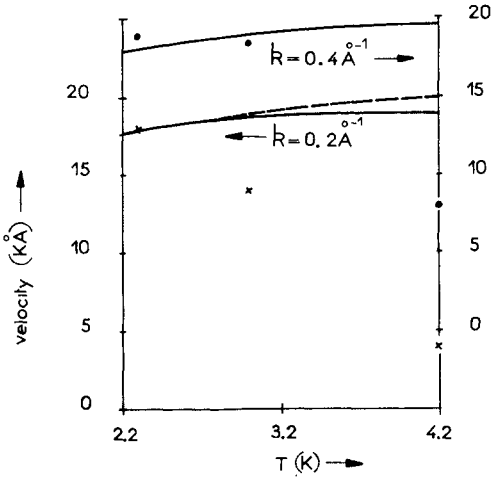

FIG. 1. The velocities of the collective mode in $S(k,\omega)$ are shown as a function of temperature for two wave vectors, together with the experimental data of Cowley and Woods. The solid curves are calculated with the measured saturated-vapor-pressure values of the particle density, whereas the dashed curve for $k=0.2$ Å^{-1} is for a constant particle density equal to n_λ. We exclude the critical region.

In the course of our calculations we found that the low-frequency pole, discussed earlier by two of us,[1] is overdamped. The occurrence of two poles in the RPA expression (1) can be deduced from the limiting behavior of $\chi_0(k,\omega)$, which is negative for $\omega=0$, and proportional to $1/\omega^2$ for large ω. There are therefore two poles for sufficiently large μ, but the low-frequency pole occurs near the maximum of $\mathrm{Im}\chi_0$ and is consequently overdamped. This behavior is completely analogous to the situation for the electron gas.[7] Here the high-frequency pole corresponds to the plasmon, and the low-frequency pole occurs inside the two-particle continuum and therefore produces no structure in the dielectric function.

In detail, we calculate $\chi(k,\omega)$ within the RPA approximation for the Hamiltonian

$$H=\sum_{\vec{k}}a_{\vec{k}}^{\dagger}a_{\vec{k}}(\epsilon_k-\mu)$$
$$+2V^{-1}\sum_{\vec{k},\vec{p},\vec{q}}u(\vec{q})a_{\vec{k}+\vec{q}}^{\dagger}a_{\vec{p}-\vec{q}}^{\dagger}a_{\vec{p}}a_{\vec{k}}, \quad (3)$$

where $\epsilon_k=k^2/2m$, μ is the chemical potential, a and $a^\dagger$ are Bose operators, and $u(q)$ is the Fourier transform of the pair potential. Since many of the steps in the calculation are given by Fetter and Walecka,[8] and in our earlier Letter,[1] we shall do no more than record the salient points, and give the values of the various parameters.

To calculate the density operator $n_{\vec{k}}=\sum a_{\vec{k}+\vec{q}}^{\dagger}a_{\vec{q}}$ in (2) we form the equation of motion for $a_{\vec{k}+\vec{q}}^{\dagger}a_{\vec{q}}$, and reduce each four-particle interaction term to the sum of all nonzero pairings of operators. After collecting together the various interaction terms, we can identify three types of contribution to the equation of motion. First, there is the self-energy contribution,

$$a_{\vec{k}+\vec{q}}^{\dagger}a_{\vec{q}}V^{-1}\textstyle\sum_{\vec{p}}u(p)\{f_{\vec{q}+\vec{p}}-f_{\vec{k}+\vec{q}+\vec{p}}\}, \quad (4)$$

where f_k is the Bose distribution function

$$f_k=\{\exp[\beta(\epsilon_k-\mu)]-1\}^{-1}. \quad (5)$$

We take this contribution into account by the replacement

$$\beta(\epsilon_k-\mu)\to\beta(m/m^*)\epsilon_k+\eta, \quad (6)$$

with η determined by

$$n=V^{-1}\textstyle\sum_p f_p \quad (7)$$

with $\eta = 0$ at T_λ. From the latter condition we find m^* in terms of T_λ and n_λ. Using the measured saturated-vapor-pressure values[9] we find $m^* = 1.44m$, and that η varies between zero at T_λ and 0.477 at 4.2°K.

The second contribution to the approximate equation of motion is

$$(f_{\vec{k}+\vec{q}} - f_{\vec{q}})V^{-1}u(k)\sum_{\vec{p}} a^\dagger_{\vec{k}+\vec{p}} a_{\vec{p}} \quad (8)$$

which is often referred to as the direct contribution. The third, and final, component is the exchange contribution,

$$(f_{\vec{k}+\vec{q}} - f_{\vec{q}})V^{-1}\sum_{\vec{p}} u(\vec{p}) a^\dagger_{\vec{k}+\vec{q}+\vec{p}} a_{\vec{q}+\vec{p}}. \quad (9)$$

Note that for a δ-function potential the exchange term (9) is identical with the direct term (8), and in this instance we would simply replace u in (8) by $2u$. However, to be consistent we would need also to take account of the wave-vector dependence of the self-energy contribution and not use the simple replacement (6). For this reason we neglect the exchange contribution (9), and our calculation is then, strictly speaking, a Hartree-RPA approximation.

Within these various approximations we obtain for $\chi(k, \omega)$ expression (1) with

$$\chi_0(k, \omega) = \frac{2}{V}\sum_{\vec{p}} f_p \frac{\epsilon_{\vec{k}+\vec{p}} - \epsilon_{\vec{p}}}{\omega^2 - (\epsilon_{\vec{k}+\vec{p}} - \epsilon_{\vec{p}})^2}. \quad (10)$$

The imaginary part of this expression for χ_0 can be expressed in closed form, but we recall only the limiting value,

$$\lim_{k\to 0} \mathrm{Im}\chi_0(k, sk) = -(sm^{*2}/4\pi\hbar^3) \times [\exp(\eta + \tfrac{1}{2}\beta m^* s^2) - 1]^{-1}. \quad (11)$$

This has a maximum value at a velocity $s \simeq (2\eta/m^*\beta)^{1/2}$, for temperatures $\sim T_\lambda$. The real part cannot be expressed in closed form but can be evaluated numerically from the imaginary part, either via dispersion relations, or as a power series in k^2.

In Fig. 1 we show the velocity of the collective mode in $S(k, \omega)$,[10] Eq. (2), evaluated from (1) and (10) as a function of temperature for two small values of the wave vector. The value of u was determined from the energy of the collective mode observed at 2.3°K and $k = 0.2$ Å^{-1}, and this gave a value $u = 1508$°K Å^3. The calculated velocities are seen to increase slowly with increasing temperature which is clearly at odds with the experimental data of Cowley and Woods. The discrepancy is even larger if we use a constant density instead of the observed saturated-vapor-pressure values. The dashed curve in Fig. 1 represents the energy of the peak in $S(k, \omega)$ for $k = 0.2$ Å^{-1} calculated with the constant density $n = n_\lambda$, and the upward temperature dependence is seen to to be quite pronounced. We conclude that the repulsion between the collective, RPA mode and the thermally excited states is not compensated by the change in the density with temperature. However, inclusion of the repulsion between the collective mode and the high-frequency, multiparticle states might outweigh that with the low-frequency, thermally excited states and bring the resultant calculated temperature dependence in line with that observed.

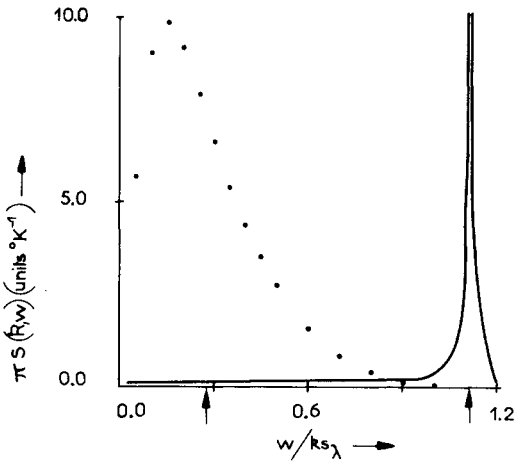

FIG. 2. The solid curve is $S(k,\omega)$ calculated for $T = 3$°K and $k = 0.2$ Å^{-1}, as a function of ω/ks_λ, where $s_\lambda = 2.17\times10^4$ cm sec^{-1}. In these units, the low-frequency pole in $\chi(k, \omega)$ occurs at 0.278 and the collective mode in $S(k,\omega)$ at 1.122, and these are denoted by arrows. The peak height in $S(k,\omega)$ is 14°K^{-1}, and has a half width at half-height of 0.025. The imaginary part of χ_0 is outlined by dots, and is seen to achieve its maximum value in the vicinity of the low-frequency pole in $\chi(k,\omega)$.

Figure 2 shows $S(k, \omega)$ for $T = 3.0$°K and $k = 0.2$ Å^{-1}, together with $\mathrm{Im}\chi_0(k, \omega)$. The half width at half-height is 0.08°K which is to be compared with the much larger experimental value of some 4°K. The major part of this discrepancy is, no doubt, due to the neglect of collisional damping. We see from Fig. 2 that there is no visible structure in $S(k, \omega)$ from the low-frequency pole in $\chi(k, \omega)$, which occurs in this instance at a velocity of 4.6°K Å. Equation (10) of Ref. 1 related the correlation energy to $S(k, \omega)$, and one might have speculated that the low-frequency mode contributed to the λ anomaly in the specific heat. From the present results, we see that this overdamped

mode can *not* make any contribution and we regretfully conclude that RPA, as we have defined it and used it in this calculation, is not even qualitatively predictive of the critical phenomena at the λ anomaly.

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[1]D. C. Mattis and L. F. Landovitz, Phys. Rev. Lett. 30, 1196 (1973).

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

[3]D. Pines, in *Quantum Fields*, edited by D. F. Brewer (American Elsevier, New York, 1966), and in *Many-Body Theory*, edited by R. Kubo (Benjamin, New York, 1966), p. 36.

[4]See, for example, W. Marshall and S. W. Lovesey, *Theory of Thermal Neutron Scattering* (Oxford Univ. Press, Oxford, 1971), Chap. 3 and Appendix B.

[5]The structure of χ_0 is discussed by D. Pines and P. Nozières, *Theory of Quantum Liquids* (Benjamin, New York, 1966).

[6]R. D. Etters, Phys. Rev. Lett. 16, 119 (1966).

[7]See, for example, Ref. 5, p. 286.

[8]A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).

[9]The energy of the collective mode in $S(k,\omega)$ is always larger than that of the pole.

[10]Thermodynamic data on liquid helium are tabulated by J. Wilks, *Properties of Liquid and Solid Helium* (Oxford Univ. Press, Oxford, 1967).