PHYSICAL REVIEW B VOLUME 33, NUMBER 1 1 JANUARY 1986

# Structure of liquid $^4$He at low temperatures: Random-phase approximation

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(Received 16 September 1985)

We have studied the enhancement of spatial order with increasing temperature in liquid $^4$He within the hypernetted-chain scheme derived from a model density matrix describing phonon and roton excitations in the liquid. The excitation spectrum was derived from the random-phase approximation (RPA) where the Bogoliubov excitations are assumed to be noninteracting. The RPA spectrum was found to be inadequate compared to the empirical spectrum, where a qualitative agreement with the experiment was found.

The prime interest in the study of liquid $^4$He at nonzero temperatures is due to the experimental observation[1,2] of a unique feature in this fluid: The short-range local order was found to be higher at finite temperature than in the ground state, and the local order is an increasing function of temperature for $T < T_\lambda$. Above $T_\lambda$ the situation is reversed. Current explanation[3-5] of this anomalous temperature dependence of the maximum of the static structure function $S(k,T)$ attributes it to thermal excitation of almost independent elementary excitations of which rotons are the dominant ones above 1 K. Reatto and his collaborators[3,4] computed the structure function $S(k,T)$ with a model density matrix, using the experimental data for the zero-temperature structure function $S(k)$ and the excitation spectrum $E_k(T)$ and observed the enhancement of short-range spatial order in the system with increasing temperature. Two of us[5] earlier extended the theoretical works of Reatto and co-workers by calculating $S(k,T)$ from the same density matrix with the hypernetted-chain (HNC) equations in the whole wave-vector range (phonons and rotons).

As mentioned above, all these theoretical works made use of the empirical excitation spectrum and are thus not entirely microscopic. The roton region of the spectrum was taken from the experimental dispersion relation measured by neutron scattering at low temperatures,[6,7] and fitted to a parabola,

$$E_k^{\rm r}(T)=\Delta(T)+\hbar^2[k-k_r(T)]^2/2\mu(T) \ , \tag{1}$$

with parameters given in Ref. 6. The small-wave-vector range of the spectrum was described by a simple phonon spectrum, $E_k^{\rm ph}(T)=\hbar c(T)k$, where $c(T)$ is the temperature-dependent speed of sound. The crossover from the phonon to the roton region was done by a simple interpolation ignoring the exact shape of the maxon part of the spectrum.

In our attempt to develop a complete microscopic approach for the structure function $S(k,T)$ at low temperatures, we have derived the excitation spectrum in the random-phase approximation (RPA). We have employed the Bose Green's function (unperturbed) in the canonical ensemble derived by Lee,[8]

$$G_0(\mathbf{p},\omega_n)=[i\omega_n-(\epsilon_p+\Delta)]^{-1} \ , \tag{2}$$

where

$$\epsilon_q=\hbar^2q^2/2m, \quad \omega_n=2\pi n/\beta, \quad \beta=1/k_BT \ ,$$

and $n$ is an integer. In Eq. (2) $\Delta$ is an infinitesimal positive constant which can be identified with the chemical potential of the ideal Bose gas. Following the diagram rules of Lee, the irreducible polarization operator $\Pi(\mathbf{p},\omega_n)$ to *leading* order is given by

$$\Pi_0(\mathbf{p},\omega_n)\equiv$$  $$=\frac{1}{\Omega}\sum_{\mathbf{q}}\frac{1}{i\omega_n-(\epsilon_{q+p}-\epsilon_q)}(N_q-N_{q+p}) \ , \tag{3}$$

where

$$N_q=-\frac{1}{\beta}\sum_n \exp(i\omega_n\eta)G_0(\mathbf{q},\omega_n)=(e^{\beta(\epsilon_q+\Delta)}-1)^{-1} \tag{4}$$

is the Bose distribution function. In obtaining Eq. (3), we have employed the standard technique of frequency summation,[9]

$$\sum_n \exp(i\omega_n\eta)/(i\omega_n-x)=-\beta/(e^{\beta x}-1) \ , \tag{5}$$

to sum over the intermediate frequencies. Rearranging the terms in Eq. (3), we obtain

$$\Pi_0(\mathbf{p},\omega_n)=(n_0-n_p)\left(\frac{1}{i\omega_n-\epsilon_p}-\frac{1}{i\omega_n+\epsilon_p}\right)+\int\frac{d^3q}{(2\pi)^3}\frac{N_q-N_{p+q}}{i\omega_n-(\epsilon_{q+p}-\epsilon_q)} \ , \tag{6}$$

where $n_0=N_0/\Omega$, $n_p=N_p/\Omega$, and $\sum_{\mathbf{q}(\neq 0,-\mathbf{p})}$ has been written as integrations.

In our present calculation, we retain only the *leading* term,

$$\Pi^{(0)}(\mathbf{p},\omega_n)=n_0\left(\frac{1}{i\omega_n-\epsilon_p}+\frac{1}{-i\omega_n-\epsilon_p}\right) \ . \tag{7}$$

As Lee pointed out, in this approximation the system could be regarded as a collection of noninteracting Bogoliubov excitations. In this case, the *chain* summation with the bare interaction in momentum space, $v_p$ (dashed line), as the driving term is calculated as

$$C(\mathbf{p},\omega_n)=$$  $$=\frac{v_p^2\Pi^{(0)}}{1-v_p\Pi^{(0)}}=\frac{2n_0v_p^2\epsilon_p}{(i\omega_n-E_p)(i\omega_n+E_p)} \ , \tag{8}$$

 

where $E_p=(\epsilon_p^2+2n_0v_p\epsilon_p)^{1/2}$ is the Bogoliubov energy.

The static structure function in the random-phase approximation is then obtained from[10–12]

$$S(\mathbf{p})=-\frac{1}{n_0\beta}\sum_n\frac{\Pi^{(0)}(\mathbf{p},\omega_n)}{1-v_p\Pi^{(0)}(\mathbf{p},\omega_n)}=\frac{\epsilon_p}{E_p}\coth(\tfrac{1}{2}\beta E_p)\ . \tag{9}$$

The HNC equation for the radial distribution function is[5]

$$g(r,T)\simeq\exp[u_2^0(r)+u_2^T(r)+N(r,T)]\ ,$$

with

$$N(r,T)=\int\frac{d^3k}{(2\pi)^3}\frac{[S(k,T)-1]^2}{\rho S(k,T)}e^{i\mathbf{k}\cdot\mathbf{r}}\ , \tag{10}$$

and the ground-state correlation factor $u_2^0(r)$. The temperature-dependent correlation function,

$$u_2^T(r)=-\int\frac{d^3k}{(2\pi)^3}\frac{2\chi_k}{1+\chi_k}\frac{1}{\rho S(k)}e^{i\mathbf{k}\cdot\mathbf{r}}\ ,$$
$$\chi_k=\exp[-\beta E_k(T)]\ , \tag{11}$$

was obtained from a model density matrix that incorporates the Landau picture of superfluid $^4$He in terms of a gas of almost independent elementary excitations and the Feynman picture of a roton as a density oscillation. These HNC equations are now solved together with the RPA equation for the excitation spectrum

$$E_k=\frac{\hbar^2k^2}{2mS(k,T)}\coth(\tfrac{1}{2}\beta E_k)\ . \tag{12}$$

At $T=0$, we recover from Eq. (12) the familiar Bijl-Feynman excitation energy, $E_k=\hbar^2k^2/2mS(k)$. Also, equating these two excitation energies, we obtain the so-called Feenberg expression[13]

$$S(k,T)=S(k)\coth(\tfrac{1}{2}\beta E_k)\ . \tag{13}$$

It is interesting to note that Ristig, Senger, Kürten, and Campbell have recently obtained a similar expression Eq. (12) for the excitation energy, by varying the trial free energy and employing the separability assumption.[14]

In Fig. 1 we have plotted $\Delta S=S(k,\ T=1.97\ \text{K})-S(k,\ T=0\ \text{K})$ as a function of the wave vector obtained from the HNC equations, Eqs. (10) and (11), with two different excitation energies: the interpolation of the experimental data as in Eq. (1) (solid line) and the RPA excitation energies as in Eq. (12) (dashed line). In the former case, the results are in qualitative agreement with experimental results for $\Delta S$ (plotted as dots in Fig. 1). In contrast, results for the RPA spectrum do not show any enhancement at all. The reason for this inadequacy could perhaps be traced in Fig. 2, where the two excitation energies at $T=1.97$ K are plotted. For $k\leq1$ Å$^{-1}$, the two results are comparable. However, the roton minimum in the RPA (dashed line) is about three times larger than that in the interpolared curve of the experimental data (solid line). The region of the roton minimum happens to be the region where the enhancement in the $\Delta S$ is expected. In fact, in the roton region, the RPA spectrum does not even have qualitatively correct temperature dependence, since it increases with increasing temperature[14] while the experimental spectrum decreases. The shift in the roton

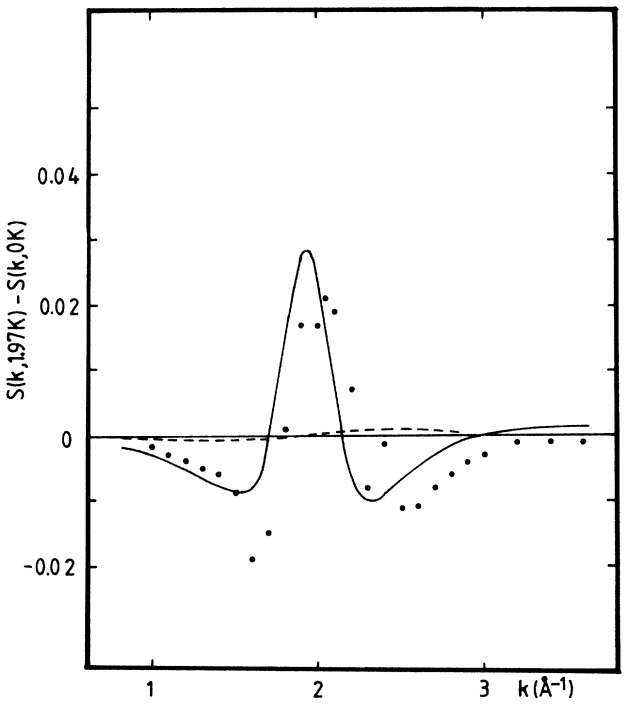


FIG. 1. Temperature effect, $\Delta S(k,T)=S(k,T=1.97\ \text{K})-S(k,T=0\ \text{K})$ at $\rho=\rho_{eq}$, with the interpolated experimental spectrum (solid line) and the RPA excitation energy (dashed line). The dots are the experimental results.

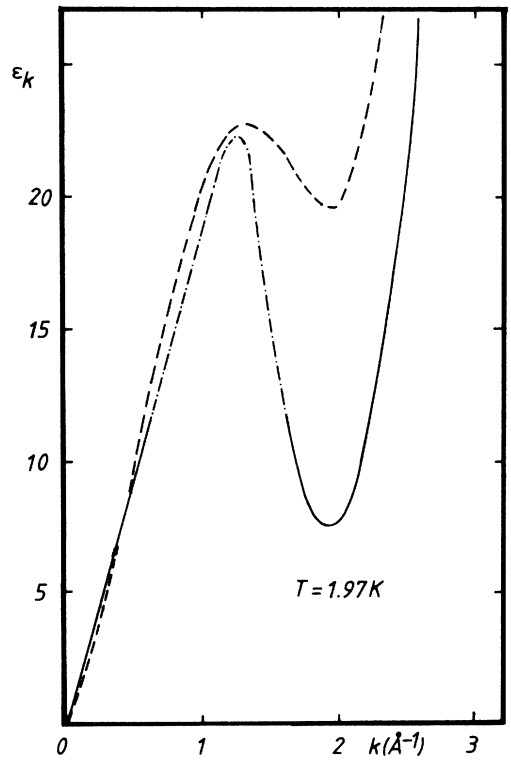


FIG. 2. Excitation spectrum at $T=1.97$ K and $\rho=\rho_{eq}$. The interpolated curve from the experimental data (solid line) and the RPA result (dashed line). The dot-dashed region of the experimental curve has not been interpolated correctly [see discussion below Eq. (1)].

gap is usually attributed to a roton-roton interaction,[15] which is not considered in the present work. For small wave vectors, however, RPA results agree quite well with the experimental data even at finite temperatures.[13,14]

In a future attempt to improve the present discrepancy, one must incorporate the rest of the *bubble* diagrams of higher order, in addition to the integral term ignored in Eq. (6). In fact, to the leading order considered in the present work, the depletion of the condensate due to particle interaction is not taken into account. Interactions among the Bogoliubov excitations should be taken into account by incorporating diagrams of the type[8,10]

where the wiggly lines represent the effective potential

$$v_{\text{eff}}(\mathbf{p},\omega_n)=v_p+C(\mathbf{p},\omega_n) \quad . \tag{14}$$

Such calculations, though involved, are invariably needed in order to achieve the desired enhancement in the spatial order from a purely microscopic standpoint.

One of us (T.C.) wishes to thank J. C. Lee for sending him papers on the thermal Green's function, and M. L. Ristig for discussions. He also acknowledges financial support by the Research Institute of Theoretical Physics, University of Helsinki and the Nordisk Institut for Teortisk Atomfysik, Copenhagen.

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