Characteristics of the dynamic structure factor of a weakly imperfect Bose gas

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(Submitted 18 February 1992)
Zh. Eksp. Teor. Fiz. **102**, 107–119 (July 1992)

We show that the results of the theory of a degenerate weakly imperfect Bose gas, including an expression for the spectrum of the eigenmodes and the free energy can be obtained from the usual diagram technique in which one uses a single-particle distribution, taking into account the presence of a Bose condensate. Within the approach developed here the dynamic structure factor of a weakly imperfect Bose gas at a finite temperature has an additional maximum in the vicinity of the $\hbar\omega = \varepsilon_k$ curve which agrees with the experimental results for superfluid helium.

1. The presently available microscopic theory of a weakly imperfect Bose gas is based upon Refs. 1 and 2, where in the $T = 0$ case a special approach was developed for the single-particle Green functions; it was connected with separating the consideration of the particles in the Bose condensate and in the supercondensate states. The detailed analysis of the corresponding results and the special diagram technique have been expounded in detail in review articles[3,4] and monographs.[5–7] At the same time, it is well known that the need to take the Bose condensate into account is shown by an analysis of the single-particle distribution function of a perfect Bose gas at arbitrary temperatures. Moreover, there is a unique expression for that function also at temperatures below the Bose condensation temperature. From that point of view it seems reasonable to apply the usual perturbation theory diagram technique taking into account the influence of the Bose condensation at the level of the single-particle distribution function.[8]

Another important point is that by now we have detailed information about the spectrum of the eigenmodes in superfluid helium (see Ref. 9). This information was obtained from the data about the maxima of the dynamic structure factor $S(k,\omega)$ for fixed values of the wave vector k. This means, in particular, that the known single-roton curve characterizes the pole of the "density-density" Green function, and not that of the single-particle Green function. This fact was taken into account in Refs. 10 to 13 where the "density-density" Green function was also considered on the basis of a special diagram technique. However, there exists within the framework of the usual diagram technique a well-known permittivity formalism which has been successfully used for a study of the spectra of eigenmodes in condensed media.[14,15]

Finally, the dynamic structure factor measured in superfluid helium has one special feature. Apart from the maxima connected with the phonon-roton spectrum and the two-roton state,[16] yet another much less pronounced maximum was observed, the position of which is well described by the energy curve of a free helium atom.[17,18] If one assumes that this maximum corresponds to a well defined eigenmode branch, it is clear that this will contradict Landau's condition for the existence of superfluidity. To explain this maximum one therefore used a statement such as a local violation of superfluidity.[19] As a result, a special experiment was carried out[20] and its authors stated that there was no such maximum. However, an analysis of the results given in Ref. 20 enabled one to speak only of a possible shift of its position.

In the present paper we show that the classical results of the theory of a degenerate weakly imperfect Bose gas, including an expression for the eigenmode spectrum and the free energy, can be obtained applying the usual temperature diagram technique, taking into account the effect of the Bose condensation at the level of the single-particle distribution function. A numerical analysis of the expressions obtained for the dynamic structure factor at finite temperatures enables us to explain the experimental features of the $S(k,\omega)$ function in superfluid helium.

2. We consider a many-body system of density n at a temperature T which consists of interacting zero-spin Bose particles and which is characterized by the Hamiltonian

$$\hat{H}=\sum_{\mathbf{p}}\varepsilon_{\mathbf{p}}\hat{a}_{\mathbf{p}}^{+}\hat{a}_{\mathbf{p}}+\frac{1}{2V}\sum_{\mathbf{p}_1\mathbf{p}_2\mathbf{k}}v(\mathbf{k})\hat{a}_{\mathbf{p}_1}^{+}\hat{a}_{\mathbf{p}_2}\hat{a}_{\mathbf{p}_2+\mathbf{k}}^{+}\hat{a}_{\mathbf{p}_1-\mathbf{k}}. \tag{1}$$

Here $\hat{a}_p^+$ and $\hat{a}_p$ are, respectively, the creation and annihilation operators of particles with momentum $\hbar p$,

$$\hat{a}_{\mathbf{p}_1}\hat{a}_{\mathbf{p}_2}^{+}-\hat{a}_{\mathbf{p}_2}^{+}\hat{a}_{\mathbf{p}_1}=\delta_{\mathbf{p}_1,\mathbf{p}_2},$$
$$\varepsilon_p=\hbar^2p^2/2m, \qquad v(k)=\int d\mathbf{r}\exp(-i\mathbf{kr})v(r), \tag{2}$$

m is the particle mass, $v(r)$ is the interparticle interaction potential, and V is the volume of the system.

By definition the dynamic structure factor is equal to[7]

$$S(k,\omega)=V^{-1}\int_{-\infty}^{\infty}dt\exp(i\omega t)\langle\delta\hat{n}_{\mathbf{k}}(t)\delta\hat{n}_{-\mathbf{k}}(0)\rangle, \tag{3}$$

where

$$\delta\hat{n}_{\mathbf{k}}(t)=\int d\mathbf{r}\exp(-i\mathbf{kr})\delta\hat{n}(\mathbf{r},t), \qquad \delta\hat{n}(\mathbf{r},t)=\hat{n}(\mathbf{r},t)-n$$

is the operator of the particle-number density fluctuations in the Heisenberg representation and $\langle\cdots\rangle$ is an average over a grand canonical Gibbs ensemble with the exact Hamiltonian $\hat{H}$ of (1). The dynamic structure factor $S(k,\omega)$ of (3) is directly connected with the retarded "density-density" Green function $L^R(k,z)$ which is analytical in the upper complex z half-plane.[7]

 0038-5646/92/070056-07$05.00

$$S(k,\omega)=-2\hbar\left\{1-\exp\left(-\frac{\hbar\omega}{T}\right)\right\}^{-1}\operatorname{Im}L^R(k,\omega+i0), \quad (4)$$

$$L^R(k,z)=-\frac{i}{\hbar V}\int_0^\infty dt\exp(izt)\langle[\delta\hat{n}_k(t),\delta\hat{n}_{-k}(0)]\rangle$$

$$\equiv V^{-1}\langle\langle\delta\hat{n}_k|\delta\hat{n}_{-k}\rangle\rangle_z, \quad \operatorname{Im}z>0. \quad (5)$$

The definitions (3) and (5) must be understood in the thermodynamic limit: $V\to\infty$, $N\to\infty$, $n=N/V=$ const, where N is the average total number of particles in the system.

Equation (4) is the basis for the evaluation of the function $S(k,\omega)$ for quantum systems, using perturbation theory diagram technique methods.[15] The retarded Green function $L^R(k,z)$ of (5) is the analytical continuation of the appropriate temperature Green function $L^T(k,i\Omega_n)$,

$$L^T(k,i\Omega_n)=V^{-1}\langle\langle\delta\hat{n}_k|\delta\hat{n}_{-k}\rangle\rangle_{i\Omega_n} \quad (6)$$

with a discrete set of points, $i\Omega_n=i2\pi nT$, on the imaginary axis, onto the upper complex z half plane.[5] We can write down a diagram representation for the function $L^T(k,i\Omega_n)$ which is connected with splitting off the so-called polarization operator[21] $\Pi(k,i\Omega_n)$ which is the irreducible part in the "k channel" with respect to a single interaction line $\nu(k)$ (see Appendix)

$$L^T(k,i\Omega_n)=\Pi(k,i\Omega_n)+\Pi(k,i\Omega_n)\nu(k)L^T(k,i\Omega_n). \quad (7)$$

After analytical continuation it follows from (7) that

$$L^R(k,z)=\Pi(k,z)/\varepsilon(k,z), \quad (8)$$

where the function $\varepsilon(k,z)$ is called the dielectric permittivity (by analogy with the terminology used in plasma theory),

$$\varepsilon(k,z)=1-\nu(k)\Pi(k,z). \quad (9)$$

Hence, using (4), we have

$$S(k,\omega)=-\frac{2\hbar}{1-\exp(-\hbar\omega/T)}\frac{\operatorname{Im}\Pi(k,\omega+i0)}{|\varepsilon(k,\omega+i0)|^2}. \quad (10)$$

It follows from (10) that the function $S(k,\omega)$ has a well defined maximum for a given value of the wave vector k in the range of frequencies ω where

$$|\nu(k)\operatorname{Im}\Pi(k,\omega+i0)|\ll 1, \quad (11)$$

$$\operatorname{Re}\varepsilon(k,\omega+i0)=0, \quad (12)$$

However, it is well known from the theory of plasma systems,[15] that Eqs. (11) and (12) are, respectively, the condition for the existence of and the dispersion equation for the longitudinal density eigenmodes. One can easily verify this by taking it into account that when a weak scalar field $\varphi^{ext}(\mathbf{r},t)$ acts on the system the average density fluctuation $\delta n(\mathbf{r},t)$ is determined by the relation (in fourier components)[7]

$$\delta n(\mathbf{k},\omega)=L^R(k,\omega+i0)\varphi^{ext}(\mathbf{k},\omega). \quad (13)$$

The pole of the Green function $L^R(k,z)$ in the lower complex z half-plane will thus determine the temporal behavior of the average density fluctuation.

It follows from (8) that the pole of the function $L^R(k,z)$ can be found from the dispersion equation

$$\varepsilon(k,z)=0, \quad (14)$$

which is well known in plasma theory.[15] As usual, one can only speak of an eigenmode spectrum if the eigenmodes are well defined:

$$|\operatorname{Im}z(k)/\omega(k)|\ll 1, \quad \omega(k)=\operatorname{Re}z(k). \quad (15)$$

If we use (15), the dispersion relation (14) takes the form

$$\operatorname{Re}\varepsilon(k,\omega(k))=0, \quad (16)$$

$$\operatorname{Im}z(k)=-\left\{\frac{\partial\operatorname{Re}\varepsilon(k,\omega)}{\partial\omega}\right\}^{-1}\operatorname{Im}\varepsilon(k,\omega)|_{\omega=\omega(k)}, \quad (17)$$

which is completely equivalent to conditions (11) and (12) for the existence of a well defined maximum of the function $S(k,\omega)$. The position $\omega_{\max}(k)$ of the function $S(k,\omega)$ can thus characterize the spectrum $\omega(k)$ of the eigenmodes in the system considered only if conditions (11) and (15) are satisfied. In experimental studies the condition (15) is usually treated as stating that the halfwidth of the maximum is small as compared to the value of $\omega_{\max}(k)$.

We note further the possibility of a nonmonotonic behavior of the function $S(k,\omega)$ which is not connected with the existence of eigenmodes in the system. The corresponding maxima will no longer satisfy the condition that they are well defined. Moreover, their occurrence is caused just by the violation of relation (11). We are dealing with the so-called "strong absorption" region where

$$|\nu(k)\operatorname{Im}\Pi(k,\omega+i0)|\gg 1. \quad (18)$$

It follows from (10) that in this frequency range the dynamic structure factor $S(k,\omega)$ will have a local minimum in the vicinity of which inevitably a maximum appears since the function $S(k,\omega)$ has the following properties:

$$S(k,\omega)\geqslant 0, \quad S(k,\omega)\underset{\omega\to\infty}{\longrightarrow}0. \quad (19)$$

The frequency range (18) is clearly determined by the characteristic energy transitions in the system considered. In particular, an appropriate analysis enables us to explain the experimental data about the scattering of electron beams in metals.[14] The well defined maxima in the structure factor correspond in metals to the electron plasma modes spectrum. The region (18) is then determined by interband transitions which also lead to the appearance of maxima, but now much less pronounced than in the plasma maxima.

We shall show in what follows that a similar situation is realized in a weakly imperfect Bose gas. The position $\omega_{\max}(k)$ of the well defined maxima of the function $S(k,\omega)$ corresponds to the dispersion equation (16) and leads to the usual phonon-roton spectrum. And the "strong absorption" region (18) is here determined by the frequencies $\hbar\omega\approx\varepsilon_k$ characterizing transitions of particles from the condensate into excited states. If we take (19) into account this leads to the appearance of an additional maximum in the dynamic structure factor in the vicinity of the $\hbar\omega=\varepsilon_k$ curve, which can serve as a substantiation of the experimental results discussed in the Introduction.

3. We have noted already in Sec. 1 that we shall in the evaluation of the polarization operator $\Pi(k,z)$ apply the usual temperature diagram technique. We then consider, in our study of the weakly imperfect Bose gas, the random

phase approximation (RPA)—a simple "loop" of single-particle Green functions of a perfect gas. In that case we have[21]

$$\Pi^{RPA}(k, i\Omega_n)=\frac{1}{V}\sum_{p}\frac{f_{p-k/2}-f_{p+k/2}}{i\Omega_n+\varepsilon_{p-k/2}-\varepsilon_{p+k/2}}. \quad (20)$$

Here f_p is the momentum distribution function for the perfect Bose gas,

$$f_p=\langle \hat{a}_p^{+}\hat{a}_p\rangle^{(0)}. \quad (21)$$

The important point is to preserve the sign of the summation over the momenta. The transition to integration must be carried out only after an analysis of the distribution function, as is done in the theory of a perfect Bose gas.[5-7] We must then consider two temperature ranges.

1) $T>T_0$ where T_0 is the Bose condensation temperature of the perfect gas,

$$T_0=\frac{1}{2m}\left(\frac{4\pi^2 n}{\Gamma(3/2)\zeta(3/2)}\right)^{2/3}, \quad (22)$$

$\Gamma(x)$ is the gamma function, and $\zeta(x)$ the Riemann function. In that case the function f_p is determined by the Bose–Einstein distribution,

$$f_p=\left\{\exp\left(\frac{\varepsilon_p-\mu^0}{T}\right)-1\right\}^{-1} \quad (23)$$

with the normalization condition to determine the chemical potential μ^0,

$$n=\int\frac{d^3p}{(2\pi)^3}f_p. \quad (24)$$

It is then possible to change in (21) directly to an integration over momenta. Hence

$$\Pi^{RPA}(k, \omega+i0)=\int\frac{d^3p}{(2\pi)^3}\frac{f_{p-k/2}-f_{p+k/2}}{\hbar\omega+\varepsilon_{p-k/2}-\varepsilon_{p+k/2}+i0}. \quad (25)$$

2) $T\leqslant T_0$. In that case the chemical potential μ^0 of the perfect Bose gas is equal to zero and the distribution function is determined by the relation[22]

$$f_p=N_0\delta_{p,0}+f_p^{T}(1-\delta_{p,0}), \quad (26)$$

$$f_p^{T}=\{\exp(\varepsilon_p/T)-1\}^{-1}, \quad (27)$$

and N_0 is the number of particles in the Bose condensate,

$$N_0=N\{1-(T/T_0)^{3/2}\}. \quad (28)$$

Substituting (26) into (20) we find

$$\Pi^{RPA}(k, \omega+i0)=\Pi^{0}(k, \omega+i0)+\Pi^{T}(k, \omega+i0), \quad (29)$$

$$\Pi^{0}(k, \omega+i0)=\frac{2n_0\varepsilon_k}{\hbar^2\omega^2-\varepsilon_k^2}-2\pi n_0\varepsilon_k i\delta(\hbar^2\omega^2-\varepsilon_k^2)\operatorname{sign}\omega, \quad (30)$$

$$\Pi^{T}(k, \omega+i0)=\int\frac{d^3p}{(2\pi)^3}\frac{f_{p-k/2}^{T}-f_{p+k/2}^{T}}{\hbar\omega+\varepsilon_{p-k/2}-\varepsilon_{p+k/2}+i0}$$

$$=\frac{m}{4\pi^2\hbar^2 k}\int_0^{\infty}dp\,p f_p^{T}\ln\left|\frac{\left(\frac{\hbar^2 pk}{m}-\varepsilon_k\right)^2-\hbar^2\omega^2}{\left(\frac{\hbar^2 pk}{m}+\varepsilon_k\right)^2-\hbar^2\omega^2}\right|$$

$$-\frac{im^2T}{4\pi\hbar^4 k}\ln\left|\frac{1-\exp\left[-\frac{\varepsilon_k}{4T}\left(1+\frac{\hbar\omega}{\varepsilon_k}\right)^2\right]}{1-\exp\left[-\frac{\varepsilon_k}{4T}\left(1-\frac{\hbar\omega}{\varepsilon_k}\right)^2\right]}\right|. \quad (31)$$

In the approximation considered the dynamic structure factor $S(k,\omega)$ has the form

$$S^{BG}(k, \omega)=-\frac{2\hbar}{1-\exp(-\hbar\omega/T)}\frac{\operatorname{Im}\Pi^{RPA}(k, \omega+i0)}{|1-v(k)\Pi^{RPA}(k, \omega+i0)|^2} \quad (32)$$

It follows from (27) to (31) that in the strong degeneracy limit, $T\ll T_0$, it is sufficient in the calculation of the operator Π^{RPA} to restrict oneself to taking into account merely Π^0 from (30). The position of the maximum of $S(k,\omega)$ is then determined by the dispersion relation (16) and has the well-known form

$$\hbar\omega(k)=\{\varepsilon_k^2+2nv(k)\varepsilon_k\}^{1/2}. \quad (33)$$

Applying the usual temperature diagram technique for the single-particle distribution function while taking the effect of the Bose condensate into account, thus enables us to establish a direct link with the experimental results about the positions of the maxima of the $S(k,\omega)$ function which characterize the phonon-roton eigenmode spectrum.

Moreover, according to the results obtained it is possible for us to take into account temperature effects when describing the dynamic structure factor of a weakly imperfect Bose gas. The main feature is then that

$$|\Pi^{T}(k, \omega+i0)|\underset{\hbar\omega\to\varepsilon_k}{\longrightarrow}\infty. \quad (34)$$

Hence, using (32) we have

$$S(k, \omega)\underset{\hbar\omega\to\varepsilon_k}{\longrightarrow}0. \quad (35)$$

Taking Eq. (19) into consideration we arrive at the conclusion that in the vicinity of the $\hbar\omega=\varepsilon_k$ curve the dynamic structure factor of a weakly imperfect Bose gas shows for $T<T_0$ a nonmontonic behavior (a weakly pronounced maximum). A more detailed discussion of this result will be given in what follows using numerical calculations. Here we stress merely that the maximum in the vicinity of the $\hbar\omega=\varepsilon_k$ curve can as a matter of principle not be connected with eigenmodes in the Bose gas since the condition (34) for its occurrence violates the validity of (15) to (17). The presence of such a maximum therefore does not affect the estimate for satisfying the Landau condition for the existence of superfluidity.

4. On the basis of the results obtained for the dynamic structure factor $S(k,\omega)$ and the "density-density" Green function $L^{T}(k,i\Omega_n)$ we can calculate the static structure factor $S(k)$,

$$nS(k)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}S(k, \omega)=V^{-1}\langle\delta\hat{n}_k\,\delta\hat{n}_{-k}\rangle \quad (36)$$

and the thermodynamic characteristics of a weakly imperfect Bose gas. In the strong degeneracy limit, $T\ll T_0$, this can

be done analytically.

Indeed, for $T \ll T_0$ we have according to (20) and (26)

$$\Pi^{RPA}(k, i\Omega_n) \approx \Pi^0(k, i\Omega_n) = -\frac{2n\varepsilon_k}{\Omega_n^2 + \varepsilon_k^2}. \tag{37}$$

Hence,

$$L^T(k, i\Omega_n) \approx \frac{\Pi^0(k, i\Omega_n)}{1 - v(k)\Pi^0(k, i\Omega_n)} = -\frac{2n\varepsilon_k}{\Omega_n^2 + \hbar^2\omega^2(k)}, \tag{38}$$

where $\omega(k)$ is given by Eq. (33).

Using the spectral representation for the temperature Green functions[5] one checks easily that

$$nS(k) = -T\sum_{\Omega_n} L^T(k, i\Omega_n). \tag{39}$$

Using (38) we find thus that the static structure factor $S(k)$ of a weakly imperfect Bose gas for $T \ll T_0$ is equal to

$$S(k) = \frac{\varepsilon_k}{\hbar\omega(k)} \operatorname{cth}\left(\frac{\hbar\omega(k)}{2T}\right). \tag{40}$$

From (40) follows in the $\hbar\omega(k) \gg T$ limit the well-known result[23]

$$\hbar\omega(k) = \varepsilon_k / S(k). \tag{41}$$

In the opposite limit, $\hbar\omega(k) \ll T$ we get

$$S(k) = 2\varepsilon_k T / \hbar^2\omega^2(k), \tag{42}$$

and in particular

$$\lim_{k\to 0} S(k) = T/nv(0). \tag{43}$$

Here, as usual,[1] we have

$$0 < v(0) = \lim_{k\to 0} v(k) < \infty. \tag{44}$$

Relation (43) must satisfy the general result[24] for systems with a short-range interaction potential (44)

$$\lim_{k\to 0} S(k) = nT\varkappa_T, \tag{45}$$

where $\varkappa_T = -V^{-1}(\partial V/\partial p)_T$ is the isothermal compressibility of the system. Comparing (43) and (45) and bearing in mind that the eigenmode spectrum $\omega(k)$ of (33) for small wavevectors has the form

$$\omega(k) \approx sk, \quad s = (nv(0)/m)^{1/2}, \tag{46}$$

we arrive at the conclusion that the quantity S characterizes the isothermal sound velocity.

To calculate the free energy F of a weakly imperfect Bose gas for $T \ll T_0$ we use the general relation[24]

$$F = F^{(0)} + {}^1/_2 v(0) nN - {}^1/_2 n \sum_k v(k) + {}^1/_2 n \sum_k \int_0^1 d\lambda v(k) S_\lambda(k). \tag{47}$$

Here $F^{(0)}$ is the free energy of a perfect Bose gas,[22]

$$F^{(0)} = T\sum_k \ln\left(1 - \exp\left(-\frac{\varepsilon_k}{T}\right)\right), \tag{48}$$

and $S_\lambda(k)$ is the static structure factor (40) for particles interacting according to the potential $\lambda v(k)$. Hence we find

$$\begin{aligned}\int_0^1 d\lambda v(k) S_\lambda(k) &= \frac{2T}{n} \ln\left|\frac{\exp[\hbar\omega(k)/2T] - \exp[-\hbar\omega(k)/2T]}{\exp[\varepsilon_k/2T] - \exp[-\varepsilon_k/2T]}\right| \\ &= \frac{1}{n}(\hbar\omega(k) - \varepsilon_k) + \frac{2T}{n}\ln\left(1 - \exp\left(-\frac{\hbar\omega(k)}{T}\right)\right) \\ &\quad - \frac{2T}{n}\ln\left(1 - \exp\left(-\frac{\varepsilon_k}{T}\right)\right).\end{aligned} \tag{49}$$

Substituting (48) and (49) into (47) we find for the free energy of a weakly imperfect Bose gas for $T \ll T_0$

$$\begin{aligned}F = \frac{1}{2}v(0)n^2N - \frac{1}{2}\sum_k \{\varepsilon_k + nv(k) - (\varepsilon_k^2 + 2nv(k)\varepsilon_k)^{1/2}\} \\ + T\sum_k \ln\left(1 - \exp\left(-\frac{\hbar\omega(k)}{T}\right)\right),\end{aligned} \tag{50}$$

which is exactly the same as the well-known result of Ref. 1.

It follows immediately from (50) that the chemical potential μ of a weakly imperfect Bose gas to first perturbation theory order in the interaction is equal to[1]

$$\mu = (\partial F/\partial N)_{T,V} \approx nv(0), \tag{51}$$

which corresponds to the limiting expressions (43) and (45) for the static structure factor, if we take into account the thermodynamic equation[24]

$$\varkappa_T = \frac{1}{n^2}\left(\frac{\partial n}{\partial \mu}\right)_T. \tag{52}$$

One can thus state that for a description of a weakly imperfect Bose gas below the Bose condensation temperature one can apply the usual temperature diagram technique of perturbation theory.

5. The neglect of the contribution of the function $\Pi^T(k,\omega + i0)$ of (31) to the polarization operator $\Pi^{RPA}(k,\omega + i0)$ leads, apart from the above mentioned situation in the vicinity of the $\hbar\omega(k) = \varepsilon_k$ curve, to a δ-function behavior of the $S(k,\omega)$ function:

$$S(k, \omega) \sim \delta(\omega - \omega(k)),$$

which, strictly speaking, corresponds to the $T = 0$ case. Taking into account that the temperature is finite thus leads to the necessity to take into account the function Π^T. In the present paper we have used numerical calculations for a qualitative analysis of the dynamic structure factor of a weakly imperfect Bose gas, taking into account the available experimental data for superfluid helium (see Sec. 1). We then paid special attention to the above mentioned maximum of $S(k,\omega)$ in the vicinity of the $\hbar\omega(k) = \varepsilon_k$ curve. In this connection we used in our calculations the experimental thermodynamic parameters of superfluid helium[18] and took the Bose condensation temperature T_0 to be 2.17 K. The

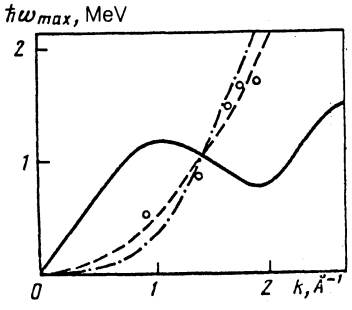

FIG. 1. Positions of the maxima of the dynamic structure factor of superfluid helium at $T = 1.2$ K. The solid line is the phonon-roton spectrum;[18] the dashed line the spectrum ε_k of a free helium atom; the dash-dot line shows the positions of the maxima of the function $S^{BG}(k,\omega)$ for a weakly imperfect Bose gas; the circles are the positions of the maxima $\omega_{max}(k)$ from Ref. 18.

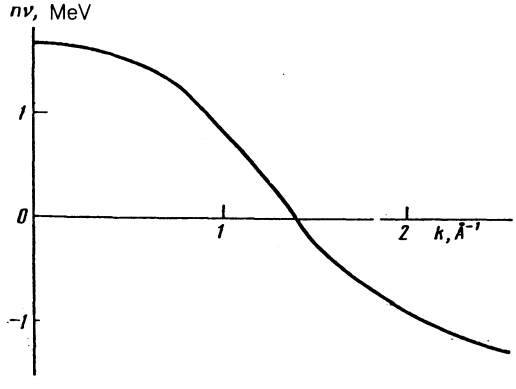

FIG. 2. Fourier component $\nu(k)$ of the interparticle interaction potential.

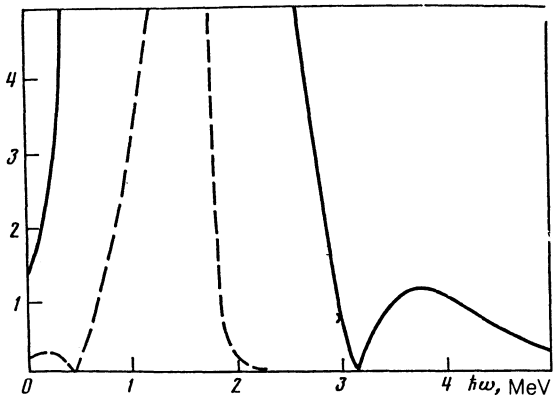

FIG. 3. Dynamic structure factor $S^{BG}(k,\omega)$ of a weakly imperfect Bose gas at $T = 1.2$ K. The dashed curves correspond to $k = 0.8$ Å^{-1}, the solid curves to $k = 2.2$ Å^{-1}.

form of the Fourier components of the interparticle interaction potential $\nu(k)$ was determined assuming that the positions of the maxima of the $S(k,\omega)$ function of superfluid helium corresponding to the experimental shape of the phonon-roton curve (Fig. 1) must correspond to the dispersion relation (16) using Π^{RPA} from (29) to (31). The corresponding results are shown in Fig. 2. The results of the numerical calculation of the dynamic structure factor $S(k,\omega)$ using Eq. (32) are shown in Fig. 3. It follows from the above consideration that the function $S(k,\omega)$ has, apart from a steep maximum corresponding to the phonon-roton spectrum, yet another not very pronounced maximum in the immediate vicinity of $\hbar\omega = \varepsilon_k$, where $S(k,\omega) = 0$. The positions of these maxima are shown in Fig. 1 and are found to be in satisfactory agreement with the experimental results.

The authors are grateful to L. P. Pitaevskiĭ and A. A. Rukhadze for their interest in this work.

APPENDIX

It is well known[5] that the fact that the average of the product of several creation and annihilation operators for a system of noninteracting particles can be reduced to products of pair averages of operators $\hat{a}_{\mathbf{p}}^{+}\hat{a}_{\mathbf{p}}$—a consequence of Wick's theorem—is the main foundation of the standard temperature diagram technique. However, when one considers a Bose gas at temperatures T below the Bose condensation temperature an arbitrarily large number of particles can be concentrated in states with zero momentum. The particle number density in the ground state ($\mathbf{p} = 0$) thus tends to a finite limit when the total number of particles N and the volume V of the system tend to infinity. This leads to the necessity to take into account averages of the normal product of the $\hat{a}_0^{+}$ and $\hat{a}_0$ operators, of the form $(\hat{a}_0^{+})^n\hat{a}_0^n$, the contribution of which is ignored in the standard temperature diagram technique. This fact was taken into account in a specially developed formalism for calculating the single-particle Green function,[2] the essence of which can be reduced to a separate consideration of two parts of this function, corresponding, respectively, to condensate particles ($g^{(0)}(p,i\omega_m)$) and to supercondensate particles ($g^{T}(p,i\omega_m)$). At the same time an analysis of the results of the application of the formalism developed in Ref. 2 for the calculation of Green functions such as the "density-density" Green function $L^{T}(k,i\Omega_n)$ of (6) shows that it is possible to use partially the rules of the standard diagram technique. In fact, we are dealing with a "correspondence rule": if in the diagram representation, for instance, for the $L^{T}(k,i\Omega_n)$ function, written down using the rules of the standard diagram technique, there are no "blocks" in which the "dangerous" $(\hat{a}_0^{+})^n\hat{a}_0^n$ products appear, this representation is valid also for temperatures below the Bose condensation temperature. In particular, the total diagram representation for the $L^{T}(k,i\Omega_n)$ Green function shown in Fig. 4 [the straight lines correspond to the exact Green functions $g(p,i\omega_m)$] is for $\mathbf{k}\neq 0$ valid for any temperature and all "dangerous" products are contained in the four-point diagram Γ. Similarly, one can for Γ write down a diagram representation which is connected with splitting off a part $\overline{\Gamma}$ which is irreducible with respect to a single interaction line in the "k channel" ($\mathbf{k}\neq 0$) [Fig. 4; the wavy line corresponds to the Fourier component $\nu(k)$ of the interparticle potential]. As a result

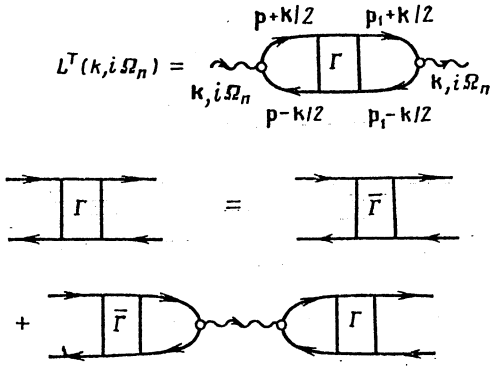

FIG. 4.

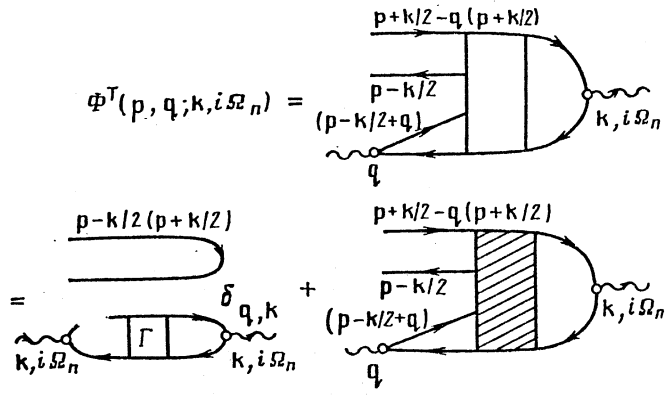

FIG. 5.

we are led to Eq. (7) for the Green function $L^T(k,i\Omega_n)$. For the known Green function $g(p,i\omega_m)$ the solution of the problem is thereby focused on the calculation of the irreducible $\overline{\Gamma}$. In the present paper we restricted ourselves to a consideration of the simplest case: $\overline{\Gamma}=\delta_{p,p_1}$ corresponding to the RPA. It is clear that in that case we have

$$\Pi^{RPA}(k,i\Omega_n)=V^{-1}\langle\langle\delta\hat{n}_k|\delta\hat{n}_{-k}\rangle\rangle^{(0)}_{i\Omega_n}, \tag{53}$$

which corresponds to (20) for all temperatures.

One can obtain a similar result also by using the exact equations of motion. Indeed, according to (6) when

$$L^T(k,i\Omega_n)=V^{-1}\sum_p F^T(\mathbf{p},\mathbf{k},i\Omega_n) \tag{54}$$

we have

$$F^T(\mathbf{p},\mathbf{k},i\Omega_n)=\langle\langle\hat{a}^+_{p-k/2}\hat{a}_{p+k/2}|\delta\hat{n}_{-k}\rangle\rangle_{i\Omega_n}. \tag{55}$$

Integrating by parts in the definition (55) of the Green function F^T and using the equations of motion for the creation and annihilation operators we find

$$i\Omega_n F^T(\mathbf{p},\mathbf{k},i\Omega_n)=\{f_{p-k/2}-f_{p+k/2}\}-(\varepsilon_{p-k/2}-\varepsilon_{p+k/2})\times F^T(\mathbf{p},\mathbf{k},i\Omega_n)+V^{-1}\sum_q v(q)\Phi^T(\mathbf{p},\mathbf{q};\mathbf{k},i\Omega_n), \tag{56}$$

$$\Phi^T(\mathbf{p},\mathbf{q};\mathbf{k},i\Omega_n)=\langle\langle\hat{a}^+_{p-k/2}\hat{n}_q\hat{a}_{p+k/2-q}-\hat{a}^+_{p-k/2+q}\hat{n}_q\hat{a}_{p+k/2}|\delta\hat{n}_{-k}\rangle\rangle_{i\Omega_n}, \tag{57}$$

where f_p is the exact single-particle distribution function. For the Green functions F^T of (55) and Φ^T of (57) one can also realize a diagram expansion connected with splitting off parts which are irreducible in the "k channel" with respect to a single interaction line. However, in this case it is necessary from the beginning to split off the unconnected parts in the Green function Φ^T (Fig. 5). This procedure is also valid at all temperatures. Hence we have

$$\Phi^T(\mathbf{p},\mathbf{q};\mathbf{k},i\Omega_n)=\{f_{p-k/2}-f_{p+k/2}\}\langle\langle\delta\hat{n}_k|\delta\hat{n}_{-k}\rangle\rangle\delta_{q,k}+\Phi^{(c)}(\mathbf{p},\mathbf{q};\mathbf{k},i\Omega_n). \tag{58}$$

The superscript (c) indicates here that the corresponding function does not contain unconnected parts. Now splitting off in the functions F^T and $\Phi^{(c)}$ the parts $\overline{F}$ and $\overline{\Phi}^{(c)}$ which are irreducible in the "k channel" with respect to a single interaction line and using (7) we obtain

$$\{i\Omega_n+\varepsilon_{p-k/2}-\varepsilon_{p+k/2}\}\overline{F}(\mathbf{p},\mathbf{k},i\Omega_n)=\{f_{p-k/2}-f_{p+k/2}\}+V^{-1}\sum_q v(q)\overline{\Phi}^{(c)}(\mathbf{p},\mathbf{q};\mathbf{k},i\Omega_n), \tag{59}$$

$$F^T(\mathbf{p},\mathbf{k},i\Omega_n)=\overline{F}(\mathbf{p},\mathbf{k},i\Omega_n)\varepsilon^{-1}(k,i\Omega_n), \tag{60}$$

$$\Phi^{(c)}(\mathbf{p},\mathbf{q};\mathbf{k},i\Omega_n)=\overline{\Phi}^{(c)}(\mathbf{p},\mathbf{q};\mathbf{k},i\Omega_n)\varepsilon^{-1}(k,i\Omega_n), \tag{61}$$

where the permittivity $\varepsilon(k,i\Omega_n)$ is given by Eq. (9). In the case of a weakly imperfect Bose gas one can clearly neglect the last term on the right-hand side of Eq. (59). As a result we again obtain

$$\Pi^{RPA}(k,i\Omega_n)=V^{-1}\sum_p\overline{F}(\mathbf{p},\mathbf{k},i\Omega_n)=V^{-1}\sum_p\frac{f^{(0)}_{p-k/2}-f^{(0)}_{p+k/2}}{i\Omega_n+\varepsilon_{p-k/2}-\varepsilon_{p+k/2}} \tag{62}$$

which confirms the validity of our considerations.

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Translated by D. ter Haar