Bose-Einstein condensation, phase fluctuations, and two-phonon effects in superfluid ^{4}He

S. Giorgini, L. Pitaevskii,* and S. Stringari
Dipartimento di Fisica, Universitá di Trento, I-38050 Povo, Italy
(Received 18 February 1992)

Various infrared divergencies characterizing the static particle Green's function and the momentum distribution of Bose superfluids are investigated through a direct analysis of the thermal and quantum fluctuations of the phase of the order parameter. We explicitly investigate the role of two-phonon effects which are responsible for logarithmic (at $T=0$) and $1/q$ (at $T\neq 0$) divergencies in the longitudinal static Green's function of a three-dimensional Bose superfluid. The temperature dependence of the condensate fraction of superfluid ^{4}He is finally discussed with special emphasis to the contribution arising from the thermal excitation of rotons.

I. INTRODUCTION

Much theoretical work has been devoted in the literature to the study of the particle Green's function of Bose superfluids (for a recent review and an up-to-date list of references see, for example, Ref. 1). Important features of such a function are associated with the occurrence of the phenomenon of Bose-Einstein condensation (BEC). In particular BEC is responsible for the existence of a discrete pole at low momenta and frequencies, corresponding to the propagation of phonons, and for the consequent appearance of infrared divergencies in the static particle Green's function as well as in the momentum distribution. The divergencies associated with one-phonon effects are well established and rather rigorously proved. These include, in particular, the $1/q$ divergency of the momentum distribution at $T=0$ (Refs. 2 and 3) and the $1/q^2$ divergency of the static Green's function.[4-9] The occurrence of additional divergencies in the longitudinal static Green's function as well as in the momentum distribution has been pointed out in Refs. 10–12 using diagrammatic analysis and functional integration methods. More recently the same problem has been investigated in Ref. 13 in the case of a dilute Bose superfluid.

The purpose of this work is to discuss the various divergencies occurring in the particle Green's function of a 3D Bose superfluid by a direct investigation of the phase fluctuations of the order parameter (Secs. III and IV). The analysis is carried out using the hydrodynamic picture of Bose superfluids which is expected to provide the correct description of infrared divergencies in interacting Bose systems. This picture allows for a natural distinction between one-phonon and two-phonon contributions and permits us in particular to calculate in a simple and transparent way the infrared divergencies arising from two phonon effects.

In Sec. V we discuss the problem of the temperature dependence of the condensate fraction $n_0(T)$. In addition to the well-known low-temperature behavior fixed by the propagation of long-wavelength phonons,[7,14] we explore the region of higher temperature and discuss the contribution to $n_0(T)$ arising from the thermal excitation of rotons.

II. STATIC PARTICLE GREEN'S FUNCTION AND MOMENTUM DISTRIBUTION

The diagonal and off-diagonal retarded particle Green's functions are defined by the equations

$$G^{a^\dagger,a}(q,\omega)=(-i)\int_{-\infty}^{+\infty}d(t-t')e^{i\omega(t-t')}\langle[\hat{a}_q^\dagger(t),\hat{a}_q(t')]\rangle\theta(t-t') , \quad (1)$$

$$G^{a,a}(q,\omega)=(-i)\int_{-\infty}^{+\infty}d(t-t')e^{i\omega(t-t')}\langle[\hat{a}_q(t),\hat{a}_{-q}(t')]\rangle\theta(t-t') , \quad (2)$$

where $\hat{a}_q(t)=e^{i\hat{H}t}\hat{a}_q e^{-i\hat{H}t}$.

In the following we will be mainly interested in the static limits $G^{a^\dagger,a}(q,\omega=0)$, $G^{a,a}(q,\omega=0)$, and in the momentum distribution of the system defined by

$$n(q)=\langle\hat{a}_q^\dagger\hat{a}_q\rangle$$
$$=-\frac{1}{\pi}\int_{-\infty}^{+\infty}d\omega\frac{1}{1-\exp(-\beta\omega)}\mathrm{Im}G^{a^\dagger,a}(q,\omega) , \quad (3)$$

where $\beta=1/k_BT$ and $\hbar=1$. Definitions (1)–(3) hold both at $T=0$ and $T\neq 0$. In the latter case the dissipation-fluctuation theorem permits us to relate the low-q limit of the above quantities through the equation

$$n(q)_{q\to 0}=-k_BTG^{a^\dagger,a}(q,\omega=0)_{q\to 0} . \quad (4)$$

At low q the behavior of the particle Green's functions (1)–(2) in a Bose superfluid is fixed by the following laws:[4-9]

$$G^{a^\dagger,a}(q,\omega=0)_{q\to 0}=-G^{a,a}(q,\omega=0)_{q\to 0}=-\frac{n_0 m^2}{\rho_s q^2}\ , \tag{5}$$

where n_0 is the condensate density ($n_0=N_0/V$) and ρ_s is the superfluid density of the system. Result (5) can be used, together with the dissipation-fluctuation relation (4), to determine the low-q behavior of the momentum distribution at finite temperature

$$n(q,T)_{q\to 0}=\frac{k_B T m^2 n_0}{\rho_s q^2}\ . \tag{6}$$

On the other hand at zero temperature the momentum distribution obeys the low-q law:[2,3],

$$n(q,T=0)_{q\to 0}=\frac{m n_0 c}{2qn} \tag{7}$$

which originates from the zero point motion of phonons. In Eq. (7) c is the sound velocity.

While results (5)–(7) are well established and have been rather rigorously proven, the occurrence of additional divergencies in the particle Green's function as well as in the momentum distribution has been the object of less systematic work in the literature. In particular an interesting question to discuss is the low-q behavior of the longitudinal static Green's function

$$G_L(q,\omega=0)=\tfrac{1}{2}[G^{a^\dagger,a}(q,\omega=0)+G^{a,a}(q,\omega=0)]=\tfrac{1}{4}G^{a^\dagger+a,a+a^\dagger}(q,\omega=0)\ . \tag{8}$$

In fact in G_L the leading terms in $1/q^2$ of Eq. (5) cancel out, differently from what happens in the transverse Green's function:

$$G_T(q,\omega=0)=\tfrac{1}{2}[G^{a^\dagger,a}(q,\omega=0)-G^{a,a}(q,\omega=0)]=\tfrac{1}{4}G^{a^\dagger-a,a-a^\dagger}(q,\omega=0) \tag{9}$$

that diverges as $1/q^2$. The divergent nature of the longitudinal component was first anticipated by Gavoret and Nozières[2] and later explored in Refs. 10–13. In the next section we provide an explicit derivation of the low-q behavior of $G_L(q,\omega=0)$ by a proper inclusion of two-phonon effects.

III. THERMAL FLUCTUATIONS OF THE PHASE

In this section we study the behavior of the momentum distribution at small momenta and finite temperature by looking at the fluctuations of the particle operator. At small momenta these are governed by the fluctuations of the phase which are responsible for the divergent behavior of $n(q)$. It is convenient to work in the coordinate space where the one-body density [Fourier transform of $n(q)$] is given by

$$\rho^{(1)}(\mathbf{r})=\langle\hat\Psi^\dagger(\mathbf{r})\hat\Psi(0)\rangle\ . \tag{10}$$

In Eq. (10) $\hat\Psi$ is the particle operator whose macroscopic component $\hat\Psi_M$ can be written as:

$$\hat\Psi_M(\mathbf{r})=\sqrt{n_0}\,e^{i\hat\Phi(\mathbf{r})}\ , \tag{11}$$

where n_0 is the condensate density and $\hat\Phi$ is the phase operator.

In the following we will consider only the contribution to $\rho^{(1)}(\mathbf{r})$ arising from fluctuations of the phase $\hat\Phi$ which fix the long-range behavior of $\rho^{(1)}(\mathbf{r})$. Using Eqs. (10) and (11) one can write

$$\rho^{(1)}(\mathbf{r})_{r\to\infty}=n_0\langle e^{-i[\hat\Phi(\mathbf{r})-\hat\Phi(0)]}\rangle=n_0 e^{-\langle[\hat\Phi(\mathbf{r})-\hat\Phi(0)]^2\rangle/2}\ , \tag{12}$$

where we have used the fact that the probability distribution for the occurrence of phase fluctuations is Gaussian. The phase fluctuations induce changes in the grand canonical potential through the changes in the superfluid kinetic energy $K_s=\int\frac{1}{2}\rho_s v_s^2 dV$ with $\mathbf{v}_s=\nabla\Phi/m$. As a consequence the explicit form of the probability distribution is given by

$$P(\delta\Phi)\propto\exp\left[-\frac{\delta\Omega}{k_B T}\right]=\exp\left[-\frac{K_s}{k_B T}\right]=\exp\left[-\frac{\rho_s}{2m^2 k_B T}\sum_k k^2|\delta\Phi_{\mathbf{k}}|^2\right]\ , \tag{13}$$

where we have decomposed the phase fluctuation in its Fourier components. The above expression for the superfluid kinetic energy is meaningful only in the framework of the hydrodynamic picture of superfluids and consequently only for the small-k components of the phase fluctuations. From Eq. (13) we find $\langle|\delta\Phi_{\mathbf{k}}|^2\rangle=k_B T m^2/\rho_s k^2$ and for a 3D system

$$\langle\hat\Phi(\mathbf{r})\hat\Phi(0)\rangle_{r\to\infty}=\frac{k_B T m^2}{4\pi\rho_s r} \tag{14}$$

and consequently the asymptotic behavior of the one-body density takes the form

$$\rho^{(1)}(r)_{r\to\infty}=n_0\left[1+\frac{k_B T m^2}{4\pi\rho_s r}+\frac{1}{2}\left[\frac{k_B T m^2}{4\pi\rho_s r}\right]^2+\cdots\right]\ . \tag{15}$$

The factor $e^{-\langle[\hat\Phi(0)]^2\rangle}$ [see Eq. (12)] gives a renormalization of the condensate density n_0. This renormalization is fixed by short-range effects and cannot be calculated in this approach. In momentum space Eq. (15) yields

$$n(q)_{q\to 0}=\frac{n_0 m^2 k_B T}{\rho_s q^2}+\frac{n_0 m^4 (k_B T)^2}{16\rho_s^2 q}+\cdots\ . \tag{16}$$

Result (16) generalizes the well-known Equation (6) through the inclusion of the divergent term in $1/q$ whose origin, as we shall see more explicitly in the next section, can be associated with two-phonon effects. Using the fluctuation-dissipation theorem (4), result (16) yields the following low-q behavior of the static particle Green's functions:

$$G^{a^\dagger a}(q,\omega=0)_{q\to 0}=-\frac{n_0m^2}{\rho_s q^2}-\frac{k_BT}{q}\frac{m^4n_0}{16\rho_s^2}\ ,$$
$$G^{aa}(q,\omega=0)_{q\to 0}=\frac{n_0m^2}{\rho_s q^2}-\frac{k_BT}{q}\frac{m^4n_0}{16\rho_s^2}\ , \tag{17}$$

where the result for G^{aa} is straightforwardly obtained starting from the calculation of $\langle\hat{\Psi}(\mathbf{r})\hat{\Psi}(0)\rangle$.

Results (17) show that the longitudinal Green's function exhibits a $1/q$ divergency:

$$G_L(q,\omega=0)_{q\to 0}=-\frac{k_BT}{q}\frac{m^4n_0}{16\rho_s^2}\ . \tag{18}$$

The occurrence of such a behavior was already pointed out in Refs. 12 and 13. The authors of Ref. 12 did not however calculate explicitly the coefficient of the corresponding law, while the results of Ref. 13 concern the dilute Bose gas at low temperature ($n_0=n$, $\rho_S=mn$). (Note that the results of Ref. 13 differ by a factor 4 from the ours both at $T\neq 0$ [Eq. (18)] and at $T=0$ [see Eq. (28) below].)

IV. QUANTUM FLUCTUATIONS OF THE PHASE

Results (16)–(18) give the behavior of the momentum distribution and of the static particle Green's function in the "classical" regime dominated by thermal fluctuations. This regime is fixed by the condition $k_BT\gg\omega(q)$, where $\omega(q)$ gives the elementary excitation spectrum of the system. In superfluid ^{4}He this condition is in practice equivalent to imposing $k_BT\gg cq$ where c is the sound velocity.

In the opposite limit $k_BT\ll cq$ the behavior of the momentum distribution and of the static Green's function is dominated by the role of quantum fluctuations. In order to explore this "degenerate" regime, as well as the interpolation between the two regimes, we make explicit use of hydrodynamic picture of superfluids. This picture assumes that the many-body system can be replaced by a gas of noninteracting phonons and is consequently described by the hydrodynamic energy functional:

$$E=\int dV\left[\frac{\rho_0 v_s^2}{2}+\frac{\rho'^2c^2}{2\rho_0}\right]\ , \tag{19}$$

where the velocity field of the superfluid is fixed by the irrotational law $\mathbf{v}_s=\nabla\varphi$ and $\rho'=\rho-\rho_0$ is the change with respect to the equilibrium density of the system.

By quantizing the fields φ and ρ' we can introduce the hydrodynamic Hamiltonian

$$H=\sum_{\mathbf{k}}ck(\hat{c}_{\mathbf{k}}^\dagger\hat{c}_{\mathbf{k}}+\tfrac{1}{2})\ , \tag{20}$$

where $\hat{c}_{\mathbf{k}}^\dagger(\hat{c}_{\mathbf{k}})$ are the creation (annihilation) operators relative to the phonon carrying impulse $\mathbf{k}$ and frequency $\omega(k)=ck$. These operators are related to the operators $\hat{\varphi}$ and $\hat{\rho}'$ through the expressions[15,16]

$$\hat{\varphi}(t,\mathbf{r})=\sum_{\mathbf{k}}\left[\frac{c}{2V\rho_0k}\right]^{1/2}(\hat{c}_{\mathbf{k}}e^{i[\mathbf{kr}-\omega(k)t]}+\hat{c}_{\mathbf{k}}^\dagger e^{-i[\mathbf{kr}-\omega(k)t]})\ ,$$
$$\hat{\rho}'(t,\mathbf{r})=\sum_{\mathbf{k}}i\left[\frac{\rho_0k}{2Vc}\right]^{1/2}(\hat{c}_{\mathbf{k}}e^{i[\mathbf{kr}-\omega(k)t]}-\hat{c}_{\mathbf{k}}^\dagger e^{-i[\mathbf{kr}-\omega(k)t]})\ . \tag{21}$$

Similarly to Sec. II, the link between the phonon description and the formalism of particle operators is obtained using the relation $\hat{\varphi}(\mathbf{r})=\hat{\Phi}(\mathbf{r})/m$ between the velocity potential and the phase operator $\hat{\Phi}$ of the macroscopic component (11) of the particle operator.

The applicability of the above formalism is limited to the regime of low temperature, where the whole system is superfluid ($\rho_s=\rho$), and of large wavelengths, where the behavior of the quantities (1)–(3) is dominated by the phase fluctuations of the order parameter.

By expanding the exponential (11) up to second-order terms in $\hat{\Phi}$ and taking the Fourier transformation of the particle operator $\hat{\Psi}(\mathbf{r})$, one finds

$$\hat{a}_{\mathbf{q}}=\sqrt{n_0V}\,\delta_{\mathbf{q},0}+i\sqrt{n_0}\,\hat{\Phi}_{\mathbf{q}}-\frac{1}{2}\frac{\sqrt{n_0}}{\sqrt{V}}\sum_{\mathbf{p}}\hat{\Phi}_{\mathbf{p}}\hat{\Phi}_{\mathbf{q}-\mathbf{p}}\ . \tag{22}$$

Higher-order terms are not expected to give rise to divergent contributions. They however provide a renormalization of the condensate density equivalent to the one discussed in Sec. II. From Eq. (21) we obtain the simple expression ($q\neq 0$)

$$\hat{\Phi}_{\mathbf{q}}=\left[\frac{mc}{2nq}\right]^{1/2}(\hat{c}_{\mathbf{q}}+\hat{c}_{-\mathbf{q}}^\dagger) \tag{23}$$

for the phase operator $\hat{\Phi}_{\mathbf{q}}$ in terms of the phonon operators $\hat{c}_{\mathbf{q}}$ and $\hat{c}_{\mathbf{q}}^\dagger$. Equations (22) and (23) permit us to write Eqs. (1)–(3) in terms of the expectation value of products of phonon operators. If one ignores interaction terms among phonons these values are straightforwardly calculated. In particular the expectation value of odd products of phonon operators identically vanishes and in the physical quantities (1)–(3) one can distinguish in a natural way between one-phonon and two-phonon contributions. The inclusion of interaction terms among phonons gives rise to higher-order effects in the final results and will be ignored in the present work.

Inserting Eqs. (22) and (23) into Eqs. (1) and (2) we find the following result for the static particle Green's function:

$$G_T(q,\omega=0)=-\frac{mn_0}{nq^2}\ , \tag{24}$$

$$G_L(q,\omega=0)=\frac{(mc^2)^2n_0}{n^2}\frac{1}{V}\sum_{\mathbf{p}}\frac{\bar{E}(p)}{\omega^2(p)}\frac{1}{\omega^2(p)-\omega^2(|\mathbf{q}-\mathbf{p}|)}\ , \tag{25}$$

where in the sum we exclude the term with $|\mathbf{p}|=|\mathbf{q}-\mathbf{p}|$.

A similar calculation yields the result

$$n(q)=n_0 mc^2 \frac{\bar{E}(q)}{n\omega^2(q)} + \frac{(mc^2)^2 n_0}{2n^2}\frac{1}{V}\sum_{\mathbf{p}} \frac{\bar{E}(p)\bar{E}(|\mathbf{q}-\mathbf{p}|)}{\omega^2(p)\omega^2(|\mathbf{q}-\mathbf{p}|)} \tag{26}$$

for the momentum distribution. If one uses the phonon dispersion $\omega(p)=cp$ the sums of Eqs. (25) and (26) contain unphysical ultraviolet divergencies that can be avoided by introducing a cutoff in the sum. The inclusion of such a cutoff does not affect the singular low-q behavior that is the object of the present investigation and for which explicit results can be derived starting from Eqs. (25) and (26). In the above equations we have introduced the thermal average energy

$$\bar{E}(p)=\omega(p)[N(p)+\tfrac{1}{2}] , \tag{27}$$

where $N(p)=\{\exp[\beta\omega(p)]-1\}^{-1}$ is the usual Bose factor. The occurrence of such a factor suggests the distinction between two different regimes.

(i) The "classical" regime $k_B T \gg cq$, dominated by thermal fluctuations, where $\bar{E}(q)=k_B T$. Carrying out explicitly the summation over $\mathbf{p}$ one straightforwardly recovers the results of Sec. II [see Eqs. (16) and (17)] under the hypothesis $\rho_s=\rho$ (notice that this hypothesis is implicitly assumed in the low-temperature description of this section).

(ii) The "degenerate" regime $k_B T \ll cq$, dominated by quantum fluctuations, where $\bar{E}(q)=\frac{1}{2}cq$ and we find the following result for the longitudinal static Green's function:

$$G_L(q,\omega=0)_{q\to 0}=\frac{m^2 c n_0}{4n^2(2\pi)^2}\ln(qL) , \tag{28}$$

where L is a constant of the order of interatomic distances ($qL \ll 1$). The coefficient of the logarithmic divergency coincides with the one first calculated by Popov[11] using a different method based on functional integration.

Similarly for the momentum distribution we obtain the result

$$n(q)_{q\to 0}=\frac{mn_0 c}{2nq}+\text{const} . \tag{29}$$

Note that differently from the "classical" regime, the only divergency characterizing the momentum distribution of a 3D superfluid arises from the one-phonon contribution (7).

It is worth noting that the new logarithmic divergency appearing in the static longitudinal Green's function is the consequence of two-phonon effects. The origin of the logarithmic divergency has a clear interpretation if one investigates the imaginary part of the longitudinal Green's function. Such a function is related to $G_L(q,\omega=0)$ and to the longitudinal component of the momentum distribution through the equations (we work here for simplicity at $T=0$):

$$G_L(q,\omega=0)=\frac{2}{\pi}\int_0^\infty d\omega \frac{1}{\omega}\mathrm{Im}G_L(q,\omega) , \tag{30}$$

$$n_L(q)=-\frac{1}{\pi}\int_0^\infty d\omega\, \mathrm{Im}G_L(q,\omega) , \tag{31}$$

where $n_L(q)=\frac{1}{4}\langle (a_{\mathbf{q}}^\dagger+a_{-\mathbf{q}})(a_{\mathbf{q}}+a_{-\mathbf{q}}^\dagger)\rangle$. Inspection of the low-$\omega$ region in the integrand of Eqs. (30) and (31) reveals the typical situation shown in Fig. 1(a) where we find a continuum of two-phonon excitations for $\omega \geq cq$ whose strength Im $G_L(q,\omega)$ approaches a constant value when $\omega \to cq$. Note that for $\omega < cq$ the strength must vanish because of the phonon gap typical of superfluids. This ω dependence of $\mathrm{Im}G_L(q,\omega)$ is actually responsible for the logarithmic contribution to $G_L(q,\omega=0)$ and explains why the two-phonon contribution does not give rise to divergent terms in the momentum distribution at $T=0$.

The analysis of the longitudinal static Green's function and of the momentum distribution at zero temperature can be naturally extended to the 2D problem. In this case one finds that the two-phonon contribution gives rise to a logarithmic divergency in the momentum distribution

$$n(q)_{q\to 0}=\frac{mn_0 c}{2nq}-\frac{m^2c^2n_0}{16\pi n^2}\ln(qL) \tag{32}$$

and to a $1/q$ divergency in the longitudinal Green's function

$$G_L(q,\omega=0)_{q\to 0}=-\frac{m^2 c n_0}{16n^2 q} . \tag{33}$$

In this case the strength $\mathrm{Im}G_L(q,\omega)$ behaves as $1/\sqrt{\omega^2-c^2q^2}$ for small q and $\omega \geq cq$ as illustrated in Fig. 1(b). [Note that the coefficient of Eq. (33) differs by a factor 2 from the one of Ref. 11).]

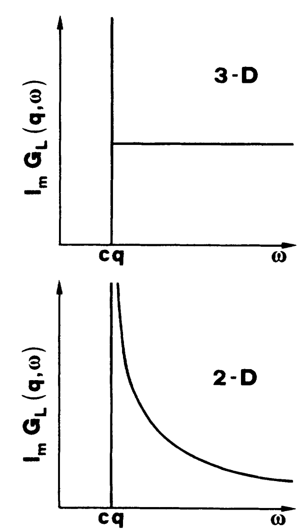

FIG. 1. Schematic picture of the longitudinal strength $\mathrm{Im}G_L(q,\omega)$ versus ω at small momenta and frequencies. Note the $1/\sqrt{\omega^2-c^2q^2}$ behavior exhibited by the two-phonon contribution to $\mathrm{Im}G_L(q,\omega)$ in the 2D case.

Direct consequences of the above results concern the behavior of the static diagonal and off-diagonal self-energies Σ_{++} and Σ_{+-} defined, for Bose systems, through the equations[16]

$$G^{aa^\dagger}(q,\omega=0)=-\frac{\frac{q^2}{2m}-\mu+\Sigma_{++}}{D}\ , \qquad (34)$$

$$G^{aa}(q,\omega=0)=\frac{\Sigma_{+-}}{D}\ , \qquad (35)$$

where

$$D=\left[\frac{q^2}{2m}-\mu+\Sigma_{++}-\Sigma_{+-}\right]\left[\frac{q^2}{2m}-\mu+\Sigma_{++}+\Sigma_{+-}\right]. \qquad (36)$$

Using the results of our analysis we find that the divergent behavior of the two-phonon contributions to the static particle Green's function implies the vanishing of the off-diagonal self-energy in 3D superfluids according to the following laws.

(i) "Classical" limit ($kT \gg cq$)

$$\lim_{q\to 0}\Sigma_{+-}=\frac{4\rho_S^2}{m^4 n_0}\frac{q}{k_B T}\ . \qquad (37)$$

(ii) "degenerate" limit ($kT \ll cq$)

$$\lim_{q\to 0}\Sigma_{+-}=\frac{n^2(2\pi)^2}{m^2 c n_0}\frac{1}{\ln(1/qL)} \qquad (38)$$

in agreement with the findings of Ref. 11.

It is finally interesting to point out that result (26) for the momentum distribution of a Bose superfluid has the same form as the one of the static structure factor in solids expanded in one-phonon and two-phonon contributions (see, for example, Ref. 17):

$$S(\mathbf{k})-S_0(\mathbf{k})=\frac{N}{m}|f(\mathbf{k})|^2 e^{-2W(\mathbf{k})}\sum_j |\mathbf{k}\cdot\mathbf{e}_j^{\mathbf{q}}|^2\frac{\bar{E}_j^{\mathbf{q}}}{\omega_j^2(\mathbf{q})}+\frac{1}{2}|f(\mathbf{k})|^2 e^{-2W(\mathbf{k})}\sum_{\mathbf{p}}\sum_{j_1 j_2}|\mathbf{k}\cdot\mathbf{e}_{j1}^{\mathbf{p}}|^2|\mathbf{k}\cdot\mathbf{e}_{j2}^{\mathbf{q}-\mathbf{p}}|^2\frac{\bar{E}_{j1}^{\mathbf{p}}\bar{E}_{j2}^{\mathbf{q}-\mathbf{p}}}{m^2\omega_{j1}^2(\mathbf{p})\omega_{j2}^2(\mathbf{q}-\mathbf{p})}\ . \qquad (39)$$

In Eq. (39) $S_0(\mathbf{k})$ is the elastic Bragg contribution, $\mathbf{q}$ is related to the reciprocal lattice vector $\mathbf{g}$ by $\mathbf{q}=\mathbf{g}-\mathbf{k}$, $f(\mathbf{k})$ is the atomic scattering factor, $e^{-2W(\mathbf{k})}$ is the Debye-Waller factor, $\mathbf{e}_j^{\mathbf{q}}$ is the polarization vector, and j indicates the various polarizations of the phonons. At $T\neq 0$ the static structure function near the Bragg value exhibits the typical $1/q^2$ and $1/q$ divergencies due to one-phonon and two-phonon contributions, respectively. The analogy between Eq. (39) and Eq. (26) is further exploited by noting that in crystals the proper order parameter is proportional to the Debye-Waller factor and the typical energy mc^2 of superfluids is replaced by the term $|\mathbf{k}\mathbf{e}_j^{\mathbf{q}}|^2/m$.

V. TEMPERATURE DEPENDENCE OF THE CONDENSATE FRACTION

In this section we investigate the temperature dependence of the condensate density $n_0(T)$ in superfluid ^{4}He. This problem has been the object of several experimental studies via neutron-scattering measurements.[18–20] From a theoretical point of view the temperature dependence of the condensate was investigated in Refs. 7 and 14 by exploring the role of long-wavelength phonons which fix the low-temperature behavior of $n_0(T)$ [see Eq. (56) below]. More recently *ab initio* microscopic calculations of $n_0(T)$ employing realistic interatomic potentials have also became available.[21,22]

The main purpose of this section is to point out the role of the roton contribution to $n_0(T)$ employing a method similar to the one first used by Landau to calculate the roton contribution to the specific heat and to the superfluid density. This approach permits us to explore the region $T=1-1.5$ K where the deviations from the $T=0$ value of n_0 start to be appreciable. To this purpose we study the termodynamic behavior of a Bose system governed by the Hamiltonian

$$\hat{H}'(\alpha)=\hat{H}'-\frac{\alpha}{2\sqrt{V}}\int d\mathbf{r}(\hat{\Psi}+\hat{\Psi}^\dagger)$$
$$=\hat{H}'-\frac{\alpha}{2}(\hat{a}_0+\hat{a}_0^\dagger) \qquad (40)$$

obtained adding the term $-(\alpha/2)(\hat{a}_0+\hat{a}_0^\dagger)$ to the grand canonical Hamiltonian $\hat{H}'=\hat{H}-\mu\hat{N}$. The inclusion of such a field breaking the gauge symmetry of the system is a usual procedure in the theoretical study of Bose superfluids.[4,5] In the presence of the perturbation the average value $\langle\hat{a}_0\rangle$ is a real number and the following identity holds:

$$\sqrt{n_0(T)V}=\langle\hat{a}_0\rangle=-\left\langle\frac{\partial\hat{H}'(\alpha)}{\partial\alpha}\right\rangle$$
$$=-\left.\frac{\partial\Omega(\alpha)}{\partial\alpha}\right|_{\alpha=0}, \qquad (41)$$

where the grand canonical potential $\Omega(\alpha)$ has to be calculated in the ensemble relative to the Hamiltonian $\hat{H}(\alpha)$. Under the hypothesis that the termodynamics of the system is equivalent to the one of a gas of noninteracting elementary excitations, the grand canonical potential can be written as

$$\Omega(\alpha,T)=\Omega(\alpha,T=0)$$
$$+\frac{k_B TV}{(2\pi)^3}\int d\mathbf{p}\ln\{1-\exp[-\beta\epsilon(\alpha,p)]\}\ , \qquad (42)$$

where $\Omega(\alpha,T=0)$ and $\epsilon(\alpha,p)$ are, respectively, the energies of the ground state and of the elementary excitations of the system governed by the Hamiltonian $\hat{H}'(\alpha)$. By explicitly carrying out the derivative of Eq. (41) with respect to α we obtain the following result for the temperature dependence of the condensate density $n_0(T)$:

$$\sqrt{n_0(T)}=\sqrt{n_0}-\frac{\sqrt{V}}{(2\pi)^3}\int d\mathbf{p}\left.\frac{\partial\epsilon(\alpha,p)}{\partial\alpha}\right|_{\alpha=0} N(p)\ , \qquad (43)$$

where n_0 is the value at $T=0$ and $N(p)$ is the Bose factor relative to the unperturbed elementary excitations. In the region of temperatures where the thermal correction is small, Eq. (43) can be rewritten as

$$n_0(T)=n_0-\frac{1}{(2\pi)^3}\int d\mathbf{p}\,\nu(p)N(p)\ , \qquad (44)$$

where we have introduced the dimensionless quantity

$$\nu(p)=2\sqrt{n_0V}\left.\frac{\partial\epsilon(\alpha,p)}{\partial\alpha}\right|_{\alpha=0}. \qquad (45)$$

Result (44) is the analog of the most famous Landau result

$$\rho_S(T)=\rho+\frac{1}{3(2\pi)^3}\int d\mathbf{p}\,p^2\frac{\partial N(p)}{\partial\epsilon} \qquad (46)$$

for the temperature dependence of the superfluid density.

The quantity $\nu(p)$ entering Eq. (44) has an alternative microscopic interpretation. In fact the temperature dependence of the condensate density can also be written as[21]

$$n_0(T)=n_0+\frac{1}{(2\pi)^3}\int d\mathbf{p}(\langle\mathbf{p}|a_0^\dagger a_0|\mathbf{p}\rangle - \langle 0|a_0^\dagger a_0|0\rangle)N(p)\ , \qquad (47)$$

where $|\mathbf{p}\rangle$ are the elementary excitations of the system. Comparison with Eq. (44) yields

$$\nu(p)=\langle 0|a_0^\dagger a_0|0\rangle-\langle\mathbf{p}|a_0^\dagger a_0|\mathbf{p}\rangle \qquad (48)$$

and shows that $\nu(p)$ corresponds to the number of atoms leaving the condensate when an elementary excitation $|\mathbf{p}\rangle$ is created in the system.

In the limit of a dilute Bose gas (DBG) the quantity $\nu(p)$ takes the analytical expression[16]

$$\nu^{\mathrm{DBG}}(p)=\frac{\epsilon^2(p)+\epsilon_0^2(p)}{2\epsilon(p)\epsilon_0(p)}\ , \qquad (49)$$

where $\epsilon_0(p)=p^2/2m$, $\epsilon(p)=[c^2p^2+\epsilon_0^2(p)]^{1/2}$, and c is the sound velocity expressed in terms of the scattering length. The same result for $\nu(p)$ can be obtained from the calculations of Ref. 13 for the energy of the elementary excitations of a weakly interacting Bose gas in the presence of the symmetry-breaking term (40).

In the region of very low temperatures the temperature dependence of $n_0(T)$ is determined by the long-wavelength excitations of the system, similarly to what happens for the superfluid density $\rho_S(T)$. This behavior was explored in Ref. 7. Here we recover the results of Ref. 7, by calculating the energies $\epsilon(\alpha,p)$ of the elementary excitations in the framework of the hydrodynamic theory of superfluids.

By developing the particle operator (11) up to second-order terms in the phase we obtain [see Eq. (22)]

$$\hat{a}_0+\hat{a}_0^\dagger=2\sqrt{n_0V}-\frac{\sqrt{n_0}}{\sqrt{V}}\sum_{\mathbf{k}}|\hat{\Phi}_{\mathbf{k}}|^2\ . \qquad (50)$$

The corresponding term $-(\alpha/2)(\hat{a}_0+\hat{a}_0^\dagger)$ has to be added to the hydrodynamic Hamiltonian that takes the form

$$\hat{H}(\alpha)=\sum_{\mathbf{k}}\left[\frac{k^2\rho}{2m^2}|\hat{\Phi}_{\mathbf{k}}|^2+\frac{c^2}{2\rho}|\hat{\rho}_{\mathbf{k}}|^2+\frac{\alpha\sqrt{n_0}}{2\sqrt{V}}|\hat{\Phi}_{\mathbf{k}}|^2\right]\ , \qquad (51)$$

where $\hat{\Phi}_{\mathbf{k}}$ and $\hat{\rho}_{\mathbf{k}}$ are the Fourier transforms of the phase and the density operators, respectively. The presence of the term in α has a crucial consequence on the equation of continuity that takes the form

$$\frac{\partial}{\partial t}\hat{\rho}_{\mathbf{k}}=\left[\frac{k^2\rho}{m}+\frac{\alpha m\sqrt{n_0}}{\sqrt{V}}\right]\hat{\Phi}_{\mathbf{k}}\ . \qquad (52)$$

The violation of the equation of continuity is a direct consequence of the fact that the perturbation field in Eq. (40) breaks the gauge symmetry, yielding a nonconservation of the number of particles. Vice versa the Euler equation is not affected by this term and the energy of the elementary excitations is finally given by the expression

$$\epsilon(\alpha,p)=cp\left[1+\frac{\alpha\sqrt{n_0}m}{n\sqrt{V}\,p^2}\right]^{1/2}. \qquad (53)$$

The α dependence of Eq. (53) accounts, as already discussed, only for the effects of the phase fluctuations induced by the particle operators $\hat{a}_0$ and $\hat{a}_0^\dagger$ entering Eq. (40) and ignores other effects originating, for example, from the fluctuations in the density induced by such operators. The effects of the phase fluctuations are the dominant ones at small momenta and give rise to a gap in the excitation energy at $p=0$

$$\epsilon(\alpha,p=0)=c\left[\frac{\alpha\sqrt{n_0}m}{\sqrt{V}n}\right]^{1/2}. \qquad (54)$$

The occurrence of a gap in the quasiparticle spectrum induced by the inclusion of perturbation terms of this nature has been already discussed in the literature.[2,13] The quantity $\nu(p)$ entering the relevant formula (44) is easily obtained from Eqs. (45) and (54) and exhibits the divergent behavior

$$\nu(p)_{p\to 0}=\frac{cm}{p}\frac{n_0}{n}\ . \qquad (55)$$

The same divergency (with $n_0=n$) occurs in the dilute Bose gas [see Eq. (49)]. By inserting result (55) in Eq. (44) we recover the result of Refs. 7 and 14

$$\frac{n_0(T)-n_0}{n_0} = -\frac{m^2 c}{\rho(2\pi)^3}\int d\mathbf{p}\frac{1}{p}N(p) = -\frac{(mk_B T)^2}{12\rho c} \tag{56}$$

holding in the $T \to 0$ limit.

When the temperature of the system is increased the role of long-wavelength phonons becomes less and less important with respect to the one of rotons. The roton contribution to $n_0(T)$ can be investigated using the same procedure currently employed in the study of $\rho_S(T)$. In particular in the roton region the relevant p dependence in the integrals (44) and (46) comes from the Bose function $N(p)$. In the range of temperature where we can ignore the phonon contribution as well as the interaction among rotons one finds the following equations:

$$n_0(T) = n_0 - \nu(p_0) N_R(T) , \tag{57}$$

$$\rho_S(T) = \rho - \frac{p_0^2}{3kT} N_R(T) , \tag{58}$$

where

$$N_R(T) = \frac{2p_0^2(\mu k_B T)^{1/2} e^{-\beta\Delta}}{(2\pi)^{3/2}} \tag{59}$$

is the density N_R of the thermally excited rotons and p_0, μ, and Δ are the usual parameters characterizing the roton spectrum. Note the different temperature dependence in the factors proportional to $N_R(T)$ in Eqs. (57) and (58).

It is worth noting that the roton coefficient $\nu(p_0)$ cannot be safely calculated using the long-wavelength expansion (55) valid only in the phonon regime (see also the comment at the end of the section) and consequently its determination requires a fully microscopic calculation. A rough estimate of $\nu(p_0)$ can be, however, obtained by rewriting Eq. (57) in the form

$$n_0(T) = n_0 - 3\nu(p_0)\frac{k_B T}{p_0^2}\rho_n(T) , \tag{60}$$

where $\rho_n = \rho - \rho_s$ is the actual normal density of the system. In this form the law for $n_0(T)$ is expected to be more accurate than Eq. (57) at high temperatures where the interactions among the elementary excitations become important. By extrapolating result (60) up to the λ point where $n_0(T_\lambda)=0$ and $\rho_n = \rho = mn$, one finds

$$\nu(p_0) = \frac{p_0^2}{3k_B T_\lambda m}\frac{n_0}{n} \tag{61}$$

and the T dependence of the condensate fraction takes the simple form

$$n_0(T) = n_0\left[1 - \frac{T}{T_\lambda}\frac{\rho_n(T)}{\rho}\right] . \tag{62}$$

Note that the behavior of Eq. (62) near T_λ agrees with the predictions of the scaling theory for second-order phase transitions according to which n_0 and ρ_s are expected,[16] in liquid helium, to have practically the same temperature dependence in the critical region: $n_0 \sim \rho_s \sim (T_\lambda - T)^{2/3}$.

Using the theoretical value $n_0/n = 0.09$ given by Green's function Monte Carlo calculations,[23,24] Eq. (61) gives the estimate $\nu(p_0) \simeq 0.6$. A larger value $[\nu(p_0) \sim 1]$ is obtained comparing directly Eq. (60) with the experimental value[20] $\delta n_0/n_0 \simeq -0.1$ at $T = 1.5$ K. The fact that in both estimates the coefficient $\nu(p_0)$ turns out to be of the order of 1 suggests the appealing idea of a direct correspondence between the atoms that leave the condensate and the thermally excited rotons. This idea leads, via Eq. (61), to a surprising connection between the smallness of the ratio n_0/n and of the quantity $3k_B T_\lambda m/p_0^2$.

A very different picture would emerge if one tried to extrapolate the hydrodynamic result (55) to the high-momentum region. A reasonable procedure is in this case to use "dispersive hydrodynamics" where the sound velocity is momentum dependent and one finds

$$\nu^{\mathrm{HD}}(p_0) = \frac{\epsilon(p_0) m}{p_0^2}\frac{n_0}{n} \simeq 0.02 . \tag{63}$$

The discrepancy between this estimate and Eq. (61) suggests that in general one might expect two possible scenarios for the temperature dependence of n_0. In the first one, corresponding to estimate (61), this dependence is exploited over the full roton region of temperature. In the second one, corresponding to estimate (63), the temperature dependence essentially occurs in the critical region where Eq. (57) is not applicable and where $n_0(T)$ rapidly jumps to zero. Experimental data seem to confirm the first scenario.

In Fig. 2 we present the prediction of Eq. (62) together with the experimental values taken from the recent analysis of neutron-scattering data of Ref. 20. Clearly much more accurate measurements in the range $T = 1 - 1.5$ K are needed in order to check the validity of Eq. (57) and to determine the coefficient $\nu(p_0)$ with better accuracy. In this context we note that the *ab initio* calcu-

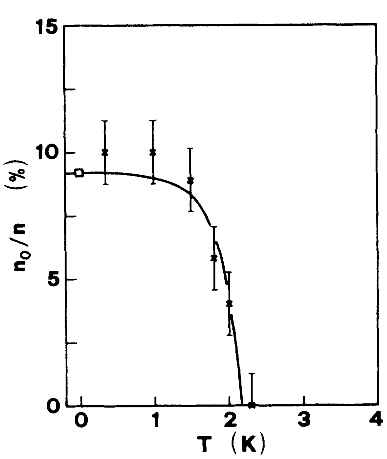

FIG. 2. Temperature dependence of the condensate fraction $n_0(T)/n$ in superfluid ^{4}He. Experimental points are taken from Ref. 20. The continuous line gives the prediction of Eq. (62).

lations of $n_0(T)$ of Ref. 22, based on a path integral Monte Carlo simulation, cannot be used to extract $\nu(p_0)$ because of the large statistical errors.

It is finally worth noting that if one neglects the possible pressure dependence of the parameter $\nu(p_0)$, Eq. (61) can be used to estimate n_0 at different pressures. The resulting predictions for $n_0(P)$ agree reasonably well with the experimental data of Ref. 20.

VI. CONCLUSIONS

In this paper we have explored in a systematic way the consequences of the thermal and quantum fluctuations of the phase of the order parameter in a 3D Bose superfluid. Such fluctuations have been shown to be at the origin of the various infrared divergencies exhibited by the static particle Green's function and momentum distribution. The method developed in this work, based on the hydrodynamic theory of superfluids, has permitted us to emphasize in a clear way the role of the elementary excitations of the system. In particular it has provided an explicit distinction between one-phonon and two-phonon contributions. The results for the two-phonon contribution to the infrared divergencies of the longitudinal static Green's function as well as of the momentum distribution have been explicitly derived and discussed at $T=0$ [Eq. (28)] and $T\neq 0$ [Eq. (16) and (18)].

We have also discussed the relevant problem of the temperature dependence of the condensate fraction. In the region of temperature where the thermodynamic behavior of the system is determined by rotons, the thermal depletion of the condensate is proportional to the density of rotons [see Eq. (57)]. A rough estimate of the coefficient of proportionality has been given. An accurate determination of this coefficient remains however an open experimental and theoretical problem.

ACKNOWLEDGMENTS

We are indebted to A. Griffin and P. Sokol for useful correspondence and discussions.

*Permanent address: Kapitza Institute for Physical Problems, ul. Kosygina 2, 117334 Moscow.

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