Condensate Density and Superfluid Mass Density of a Dilute Bose-Einstein Condensate near the Condensation Transition

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We derive via diagrammatic perturbation theory the scaling behavior of the condensate and superfluid mass density of a dilute Bose gas just below the condensation temperature, T_c. Sufficiently below T_c particle excitations are described by mean field (Bogoliubov). Near T_c, however, mean field fails, and the system undergoes a second order phase transition, rather than first order as predicted by Bogoliubov theory. Both condensation and superfluidity occur at the same T_c, and have similar scaling functions below T_c, but different finite size scaling at T_c to leading order in the system size. A self-consistent two-loop calculation yields the condensate fraction critical exponent, $2\beta \simeq 0.66$.

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The behavior of a dilute interacting homogeneous Bose gas at the condensation temperature, T_c, and in its neighborhood, is a delicate critical problem ([1–3], and references therein). Even though in a dilute gas, where $na^3 \ll 1$, with n the number density and a the s-wave particle-particle scattering length, perturbation theory fails close to T_c, and fluctuations cannot be neglected; e.g., although the shift in T_c from the free gas transition temperature, T_c^0, is linear in a, the first order perturbation result vanishes, while all higher order terms are divergent.

We calculate here the dependence on a of the condensate density, n_0, and the superfluid mass density, ρ_s, of a dilute Bose gas in three spatial dimensions, for temperatures T just below T_c, where $t \equiv (T_c - T)/T_c$ is of order a/λ. Here $\lambda = (2\pi/mT)^{1/2}$ is the thermal wavelength in units with $\hbar = 1$, and m is the particle mass. As long established, the Bogoliubov (mean field) approximation fails close to T_c; it leads to a first order phase transition (e.g., [4]) vs the second order transition expected for the universality class of the Bose gas. A similar phenomenon occurs in relativistic ϕ^4 theory [4]; a related discussion for a two dimensional Bose gas is given in Ref. [5]. We derive the general scaling structure of both n_0 and ρ_s in the critical region, as functions of t and a/λ, which connects the mean field solution to the critical behavior of a continuous phase transition. The scaling functions for n_0 and ρ_s are similar, and imply that in the (dilute) interacting Bose gas the phenomena of condensation and superfluidity occur at precisely the same temperature. A further consequence is that in the very dilute limit, $a \to 0$, where the shift of the critical temperature is linear, $T_c - T_c^0 \sim a$ [1–3,6], the condensate and superfluid mass densities at the ideal gas critical temperature, T_c^0, both vary linearly with a. We also calculate the leading order finite-size corrections to n_0 and ρ_s at T_c, which provides insight into the difference of the numerical results of Refs. [3,7] for the shift of the critical temperature.

Our approach is to study the particle densities via diagrammatic perturbation theory, working to the lowest needed order in a and n_0. To deduce the behavior of the superfluid mass density we employ Josephson's relation between ρ_s, n_0, and the long wavelength limit of the single particle Green's function [8–10].

The particle density, n, in the condensed phase is a function of a, n_0, and T, and has the form $n(a, n_0, T) = n_0 + \tilde{n}(a, n_0, T)$, where $\tilde{n}(a, n_0, T)$ is the density of noncondensed particles (with momentum $k \neq 0$). At the transition temperature, $\tilde{n}(a, 0, T_c) = n$; thus writing $\Delta\tilde{n} \equiv \tilde{n}(a, n_0, T) - \tilde{n}(a, 0, T)$, we have $n_0 + \Delta\tilde{n} = \tilde{n}(a, 0, T_c) - \tilde{n}(a, 0, T)$. Since the difference of T_c from the ideal gas transition temperature, T_c^0, is of order a [1], we may, to lowest order in a, for t of order a/λ, replace the difference on the right side by $\tilde{n}(0, 0, T_c) - \tilde{n}(0, 0, T) = n((T_c/T)^{3/2} - 1) \simeq \frac{3}{2} n\, t$. Up to corrections of order a^2, we have then

$$n_0 + \Delta\tilde{n} = \tfrac{3}{2} n\, t. \tag{1}$$

Equation (1) implicitly determines the condensate fraction, $n_0(a, t)$, as a function of a and t in the critical region, $t \lesssim a/\lambda$ or $n_0/n \lesssim a/\lambda$.

It is simplest to calculate $\tilde{n}(a, n_0, T)$ in terms of the matrix Green's function, $\mathcal{G}(rt, r't') = -i[\langle T(\Psi(rt)\Psi^\dagger(r't'))\rangle - \langle\Psi^\dagger(r't')\rangle\langle\Psi(rt)\rangle]$, where the two component field operator is $\Psi(rt) = (\psi(rt), \psi^\dagger(rt))$. The Fourier components of $\mathcal{G}^{-1}$ have the form

$$\mathcal{G}^{-1}(k, z_n) = \begin{pmatrix} z_n + \mu - \varepsilon_k - \Sigma_{11} & -\Sigma_{12} \\ -\Sigma_{21} & -z_n + \mu - \varepsilon_k - \Sigma_{22} \end{pmatrix}, \tag{2}$$

where the $z_n \equiv 2\pi i n T$ are Matsubara frequencies ($n = 0, \pm1, \pm2, \ldots$), $\varepsilon_k = k^2/2m$, and the $\Sigma_{ij}(k, z_n)$ are the corresponding self-energies. The chemical potential, μ, depends here on n_0.

The noncondensate density, $\tilde{n}$, is then found from

$$\tilde{n}(a, n_0, T) = -T\sum_n \int \frac{d^3k}{(2\pi)^3} G_{11}(k, z_n), \tag{3}$$

with

$$G_{11}(k,z) = \frac{z-\mu+\varepsilon_k+\Sigma_{22}}{(z+\mu-\varepsilon_k-\Sigma_{11})(z-\mu+\varepsilon_k+\Sigma_{22})+\Sigma_{12}\Sigma_{21}}. \tag{4}$$

Quite generally, $\Delta\tilde{n}$, to leading order in a and n_0, is given by the $z_n = 0$ contribution only:

$$\Delta\tilde{n} = -T\int \frac{d^3k}{(2\pi)^3}[G_{11}(k,0) - G(k,0)], \tag{5}$$

where $G(k,0) \equiv \lim_{n_0\to 0} G_{11}(k,0)$; integrated over k, $G(k,0)$ determines the leading order shift of the critical temperature due to interactions [1]. The Hugenholtz-Pines relation [11],

$$\mu = \Sigma_{11}(0,0) - \Sigma_{12}(0,0), \tag{6}$$

specifies μ as a function of n_0. In the zero frequency sector, $\Sigma_{11}(k,0) = \Sigma_{22}(k,0)$ and $\Sigma_{12}(k,0) = \Sigma_{21}(k,0)$, so that $\lim_{k\to 0}[(\mu - \Sigma_{11}(k,0))(\mu - \Sigma_{22}(k,0)) - \Sigma_{12}(k,0)\Sigma_{12}(k,0)] = 0$, and thus the excitation spectrum is gapless. In the following we drop the Matsubara frequency index, always referring to the zero frequency components.

The lowest order mean field self-energies, $\Sigma_{11} = \Sigma_{11}^{\rm mf} = 2g(n_0 + \tilde{n})$, $\Sigma_{12} = \Sigma_{12}^{\rm mf} = gn_0$, and $\mu = g(n_0 + 2\tilde{n})$, where $g = 4\pi a/m$, lead to the usual gapless Bogoliubov excitation spectrum. The mean field contribution to $\Delta\tilde{n}$, from Eq. (5), is

$$\Delta\tilde{n}_{mf} = -\frac{2}{\pi\lambda^2}\int dk \frac{\Sigma_{12}^{\rm mf}}{\varepsilon_k + 2\Sigma_{12}^{\rm mf}} = -\frac{2\pi^{1/2}}{\lambda^3}(n_0\lambda^2 a)^{1/2}. \tag{7}$$

Since the contribution of this term in Eq. (1) is $\propto -n_0^{1/2}$, we find two possible solutions of (1) for n_0 at the mean field critical temperature, $t_{mf} = 0$, namely $n_0 = 0$ and $n_0 = 4\pi a/\lambda^4$; intermediate values are not possible for $t > 0$. Thus Bogoliubov theory predicts a first order phase transition with a jump of the condensate density from 0 to $n_0 = 4\pi a/\lambda^4$ [4]. However, as we discuss below, mean field can be valid only outside the critical region (where $a/\lambda \ll |t| \ll 1$, and thus from Eq. (1), $a \ll n_0\lambda^4$), where it implies that $n_0 \propto t$.

To go beyond mean field we analyze the structure of the self-energies by expanding $\Sigma_{11} - \Sigma_{11}^{\rm mf}$ and $\Sigma_{12} - \Sigma_{12}^{\rm mf}$ in a series in a and the mean field Green's functions $G_{11}^{\rm mf}$ and $G_{12}^{\rm mf}$, given by Eq. (2) with the Σ_{ij} replaced by $\Sigma_{ij}^{\rm mf}$. We eliminate μ in $\mathcal{G}$ in favor of n_0 using Eq. (6). However, rather than using the gapless spectrum directly in a perturbative expansion, we write the propagators in terms of the mean field correlation length, ζ, as in [1], defined by

$$\mu - (\Sigma_{11}^{mf} - \Sigma_{12}^{mf}) = (\Sigma_{11}(0) - \Sigma_{12}(0)) - (\Sigma_{11}^{mf} - \Sigma_{12}^{mf}) \equiv -1/2m\zeta^2. \tag{8}$$

Since the propagators remain formally infrared convergent we can derive the scaling structure of the self-energies by power-counting arguments. As above the transition, the ultraviolet part, when we neglect nonzero Matsubara contributions, has only a harmless logarithmic divergence which can be removed by renormalization [1]. The expansion of the self-energies beyond mean field starts at order a^2; furthermore, Σ_{12} is formally at least of order n_0. Diagrams of order a^κ with $\kappa \geq 3$ in the formal expansion contain vertices with two Green's functions entering; similar to the structure at T_c, they involve the dimensionless combinations $a\zeta/\lambda^2$ and $n_0\lambda^2\zeta$. The latter part originates from the dependence of $\mathcal{G}^{\rm mf}$ on $2m\Sigma_{12}^{\rm mf} \sim an_0$. Any diagram with an explicit power, p, of n_0 can be generated from a corresponding diagram of power $p - 1$ in which a line is replaced by $\sqrt{n_0}$ at each of its ends. Thus each power of n_0 involves one fewer three-momentum loop to be integrated over, replacing a structure of the form $2mT\int d^3k/(k^2 + \zeta^{-2}) \sim \zeta^{-1}\lambda^{-2}$, in a loop integral of order $(a\zeta/\lambda^2)^2$, by n_0. The explicit n_0 dependences therefore enter in the combination $(a\zeta/\lambda^2)^2(n_0\zeta\lambda^2) = a^2n_0\zeta^3/\lambda^2$. Then with all momenta k scaled by $1/\zeta$, we find the following scaling structure for the self-energies:

$$\Sigma_{ij}(k) - \Sigma_{ij}^{\rm mf}(0) = T\frac{a^2}{\lambda^2}\sigma_{ij}\left(k\zeta, \frac{a\zeta}{\lambda^2}, n_0\lambda^2\zeta\right), \tag{9}$$

where the σ_{ij} are dimensionless functions of dimensionless variables. In particular, for vanishing k,

$$(\Sigma_{11}(0) - \Sigma_{12}(0)) - (\Sigma_{11}^{mf}(0) - \Sigma_{12}^{mf}(0)) = T\frac{a^2}{\lambda^2}s\left(\frac{a\zeta}{\lambda^2}, n_0\lambda^2\zeta\right), \tag{10}$$

where s is a dimensionless function.

Equations (8) and (10) imply that

$$\zeta = \frac{\lambda^2}{a}h(n_0\lambda^4/a), \tag{11}$$

where h is a dimensionless function. Then using Eqs. (9) and (11) in (5), we see that $\Delta\tilde{n}$ has the scaling structure $\Delta\tilde{n} = (a/\lambda^4)\tilde{f}(n_0\lambda^4/a)$. It immediately follows that close to T_c, where $n_0 \sim a/\lambda^4$, the dimensionless function $\tilde{f}$ cannot be determined by a perturbation expansion in $n_0\lambda^3$ or a/λ; therefore the predictions of mean field theory fail in this region. Finally from Eq. (1), using $n \sim 1/\lambda^3$ to lowest order, we derive the basic scaling result in the critical region,

$$\frac{n_0}{n} = \frac{a}{\lambda} f\left(\frac{t\lambda}{a}\right), \qquad t \lesssim \frac{a}{\lambda}, \tag{12}$$

where f is a dimensionless function. In the mean field limit, $x \to \infty$, we must have $f(x \to \infty) \sim x$, whereas the theory of critical phenomena implies a power-law behavior in the opposite limit, $f(x \to 0) \sim x^{2,\beta}$, or

$$\frac{n_0}{n} \sim \left(\frac{a}{\lambda}\right)^{1-2\beta} t^{2\beta}, \qquad \frac{t}{a/\lambda} \to 0, \tag{13}$$

where β is the critical index for the order parameter, $\langle\psi\rangle = \sqrt{n_0}$.

We see that for constant $t\lambda/a$, n_0 varies linearly with a. As $a \to 0$, T_c varies linearly in a [1]; thus at the ideal gas transition temperature $t = t_0 \equiv (T_c - T_c^0)/T_c \sim a$, for $a \to 0$, the condensate fraction varies linearly with a. This result is consistent with Leggett's weak variational bound that at t_0, n_0 is bounded above by terms of order $a^{1/3}$ [12].

We now calculate the scaling function $f(x)$ explicitly within a simple model beyond the Bogoliubov approximation. Introducing $U(k) \equiv 2m(\Sigma_{11}(k) - \Sigma_{11}(0))$, we have $\varepsilon_k + \Sigma_{11}(k) - \mu = (k^2 + U(k) + 2m\Sigma_{12})/2m$. Taking for $\Sigma_{12}(k)$ only the first order diagram in n_0, $\Sigma_{12} \equiv \Sigma_{12}^{\mathrm{mf}} = gn_0$, we may write Eq. (5) as

$$\Delta\tilde{n} \simeq -\frac{4mgn_0}{\pi\lambda^2}\int_0^\infty dk \frac{k^2}{(k^2 + U(k))(k^2 + U(k) + 4mgn_0)}. \tag{14}$$

Were we to neglect $U(k)$, we would derive the mean field result (7); rather, we determine $U(k)$ from a self-consistent two-loop calculation, as in [1],

$$U(k) = -4mg^2T^2 \int \frac{d^3q}{(2\pi)^3}\int \frac{d^3p}{(2\pi)^3} G(p+q)G(p) \times [G(k-q) - G(q)], \tag{15}$$

where $G^{-1}(k) = \mu - \varepsilon_k - U(k)/2m$ is the inverse of the ($z_n = 0$) Green's function at the transition temperature. A free particle spectrum in G would lead to a logarithmic infrared divergence. As in the calculation of the critical temperature, self-consistency of $U(k)$ at this level implies that it has the approximate structure, $U(k) = k_c^{1/2}k^{3/2}$, for nonzero $k \lesssim k_c$, with $k_c = 32(2\pi/15)^{1/2}a/\lambda^2 \approx 20.7a/\lambda^2$ [1]. A change of the power-law behavior of the free propagator to $G(k) \sim -k^{-(2-\eta)}$, for $k \to 0$, with $\eta > 0$, is possible only at precisely T_c, where the correlation length diverges. As long as $n_0 \neq 0$, the Bogoliubov operator inequality [9], $-G_{11}(k,0) \geq mn_0/nk^2$, does not permit $\eta > 0$. Therefore the $z_n = 0$ spectrum remains quadratic, $\eta = 0$, as $k \to 0$, everywhere below and above the critical temperature.

However, for $n_0\lambda^4 \ll a$, the details of the spectrum at small k do not enter, and we may approximate the self-energy as

$$U(k) = \begin{cases} k_c^{1/2}k^{3/2}: & k \ll k_c, \\ k_c^2: & k \gg k_c, \end{cases} \tag{16}$$

which in Eq. (14) leads to

$$\Delta\tilde{n} \simeq \begin{cases} (32n_0a/3k_c\lambda^2)\ln(16\pi n_0a/k_c^2): & n_0\lambda^4 \ll a, \\ -(2\pi^{1/2}/\lambda^3)(n_0\lambda^2a)^{1/2}: & n_0\lambda^4 \gg a. \end{cases} \tag{17}$$

The second line is the mean field result (7). Taken literally, this model would again predict a first order phase transition; however, the logarithmic term indicates a change in the power-law behavior close to the critical point. To determine this relation we invert Eq. (12), using $n \sim \lambda^{-3}$ to note that tn/n_0 must be a dimensionless function of the variable λ^4n_0/a. In the limit $n_0\lambda^4 \ll a$, we may write, using the upper result in Eq. (17),

$$n_0 + \Delta\tilde{n} = \frac{3}{2}nt \simeq n_0\left[1 + \frac{32a}{3k_c\lambda^2}\ln\left(\frac{16\pi n_0 a}{k_c^2}\right)\right], \tag{18}$$

which is the first term in an expansion of the scaling form

$$nt \sim n_0\left(\frac{\lambda^4 n_0}{a}\right)^{32a/3k_c\lambda^2}, \tag{19}$$

in the formal limit $a/k_c\lambda^2 \to 0$, consistent with our approximation of $U(k)$. Inverting, we derive $n_0 \sim t^{2\beta}$, with $2\beta = 1/(1 + (5/6\pi)^{1/2}) \simeq 0.66$, in excellent agreement with the value $2\beta \simeq 2/3$ expected for this universality class. In the other limit, $n_0\lambda^4 \gg a$, this model calculation simply approaches the mean field result, $n_0 \sim t$.

Below T_c the condensed system is superfluid, with a superfluid mass density, ρ_s, related to n_0 by Josephson's sum rule [8–10],

$$\rho_s = -\lim_{k\to 0}\frac{n_0m^2}{k^2G_{11}(k,0)}. \tag{20}$$

Using the explicit form (4) for $G_{11}(k,0)$, we have

$$\rho_s = n_0m + 2n_0m^2\frac{\partial}{\partial k_z^2}(\Sigma_{11}(k) - \Sigma_{12}(k))|_{k=0}, \tag{21}$$

for $T \leq T_c$. This result implies that precisely at T_c, the superfluid fraction vanishes with the condensate fraction. Above T_c, the superfluid density vanishes, as can be directly derived by calculating the transverse current-current correlation function [13].

Further, we immediately see from Eqs. (21) and (9) that the superfluid fraction in the neighborhood of the ideal gas transition has the same scaling behavior as we found for the condensate density:

$$\frac{\rho_s}{mn} = \frac{a}{\lambda}f_\rho\left(\frac{t\lambda}{a}\right), \qquad t \lesssim \frac{a}{\lambda};$$

however, the scaling function f_ρ is in general different from the scaling function f. Reference [14] obtained the scaling function for ρ_s in the dilute limit to order

$\epsilon = 4 - d$, where $d = 3$ is the spatial dimension. In the mean field limit, $t \gg a/\lambda$, the lowest order self-energies are independent of k^2, so that from Eq. (21) the superfluid mass density coincides with n_0 to order a. Thus $f_\rho(x \to \infty) \sim x$. In the critical region, however, $f_\rho(x \to 0) \sim x^\gamma$, where γ is the critical index for the superfluid mass density. Josephson's scaling relation gives $\gamma = 2\beta - \eta\nu \simeq 2/3$ for the critical index of the superfluid mass density, where $\nu \simeq 2/3$ is the critical exponent of the correlation length [8]. Since our model calculation above does not include the correct $k \to 0$ limit, to which ρ_s (but not n_0) is sensitive, it is therefore not suitable for calculating ρ_s reliably.

Let us turn to understanding the behavior of n_0 and ρ_s in large but finite systems, of linear scale L. The condensate density, $n_0^L = n - \tilde{n}^L$ at T_c, is nonzero for finite L and is found to leading order from

$$\begin{aligned} n &= n_0^\infty - T\int_0^\infty \frac{d^3k}{(2\pi)^3} G(k, \zeta) \\ &= n_0^L - T\int_{2\pi/L}^\infty \frac{d^3k}{(2\pi)^3} G(k, \zeta), \end{aligned} \tag{23}$$

where G is the infinite size Green's function. Since at T_c, $G(k \to 0) = -2mC\zeta^\eta/k^{2-\eta}$, where C is constant, and $n_0^\infty = 0$, we find,

$$n_0^L = \frac{4C}{(1+\eta)\lambda^2 L}\left(\frac{2\pi\zeta}{L}\right)^\eta, \tag{24}$$

to leading order, neglecting a numerical factor dependent on the particular geometry of the finite system. Josephson's relation should still hold inside the critical region of finite-size systems, with the limit of zero wave vector replaced by $k \to 2\pi/L$. With this relation we have

$$N^{1/3}\frac{\rho_s}{mn} = \frac{2}{(1+\eta)\lambda^2 n^{2/3}} = \frac{T_c}{T_c^0}\frac{2}{(1+\eta)\zeta(3/2)^{2/3}}, \tag{25}$$

where the total particle number is given by $N = nL^3$. Note that both Eqs. (24) and (25) are valid independent of the diluteness of the gas. Equation (25) agrees well with the numerical values of Ref. [15]. Since the limit as $a \to 0$ of η is nonzero for an interacting Bose gas, the formal $a \to 0$ limit of Eq. (25) does not, however, agree with the ideal gas value, given by the same formula but with $\eta = 0$. Therefore, the procedure of Ref. [7], to expand the finite-size scaling results directly around the ideal gas limit, is not completely justified; that there was a difficulty in this method was already suggested by the disagreement of the calculated value of $T_c - T_c^0$ with later lattice calculations [3] which do not rely on this assumption. Nevertheless, use of finite-size scaling raises new strategies for explicit calculations [16].

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[13] The vanishing of ρ_s above and at T_c follows directly from the definition of the transverse current-current correlation function. Since $G^{-1}(k \to 0) \sim k^2$ below T_c, Eq. (20) implies that both Bose condensation and superfluidity set in at the same critical temperature, T_c, for any interacting Bose fluid, not only the dilute gas. We discuss more fully, in a future publication [M. Holzmann and G. Baym (to be published)], the relation between ρ_s, n_0, and $G(k)$, as well as derive the Josephson relation from diagrammatic perturbation theory and discuss its relation to transverse current-current correlations.

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