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, $2\beta \approx 0.66$.

We calculate here the dependence on $a$ of the condensate density, $n_0$, and the superfluid mass density, $\rho_s$, of a dilute Bose gas in three spatial dimensions, for temperatures $T$ just below $T_c$, where $t = (T_c - T)/T_c$ is of order $a/\lambda$. Here $\lambda = (2\pi/mT_c)^{1/2}$ 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 $\phi^4$ 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 $\rho_s$ in the critical region, as functions of $t$ and $a/\lambda$, which connects the mean field solution to the critical behavior of a continuous phase transition. The scaling functions for $n_0$ and $\rho_s$ 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, $a \rightarrow 0$, where the shift of the critical temperature is linear, $T_c - T_0 \sim a$ [1–3,6], the condensate and superfluid mass densities at the ideal gas critical temperature, $T_0$, both vary linearly with $a$. We also calculate the leading order finite-size corrections to $n_0$ and $\rho_s$ 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 $\rho_s$, $n_0$, 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 non-condensed particles (with momentum $k \neq 0$). At the transition temperature, $\tilde{n}(a, 0, T_c) = n_0$; thus writing $\Delta \tilde{n} = \tilde{n}(a, n_0, T) - \tilde{n}(a, 0, T)$, we have $n_0 + \Delta \tilde{n} = n_0 + \tilde{n}(a, 0, T_c) - \tilde{n}(a, 0, T)$. Since the difference of $T_c$ from the ideal gas transition temperature, $T_0$, is of order $a$ [1], we may, to lowest order in $a$, for $t$ of order $a/\lambda$, replace the difference on the right side by $\tilde{n}(0, 0, T_c) - \tilde{n}(0, 0, T) = n((T_c/T)^{3/2} - 1) \approx \frac{3}{2} n_0 t$. Up to corrections of order $a^2$, we have then

$$n_0 + \Delta \tilde{n} = \frac{3}{2} n_0 t.$$  

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

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

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

where $z_n = 2\pi nT$ are Matsubara frequencies ($n = 0, \pm 1, \pm 2, \ldots$), $\epsilon_k = k^2/2m$, and the $\Sigma_{ij}(k, z_n)$ are the...
corresponding self-energies. The chemical potential, \( \mu \), depends here on \( n_0 \).

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

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

(3)

with

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

(4)

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

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

(5)

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

\[
\mu = \Sigma_{11}(0, 0) - \Sigma_{12}(0, 0),
\]

(6)

specifies \( \mu \) 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 \( \lim_{k \to 0} \mu = \Sigma_{11}(0, 0) - \Sigma_{12}(0, 0) = 0 \). Hence 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, \( \Sigma_{11} = \Sigma_{11}^{mf} = 2g(n_0 + \tilde{n}) \), \( \Sigma_{12} = \Sigma_{12}^{mf} = g n_0 \), 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

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

(7)

Since the contribution of this term in Eq. (1) is \( -n_0 \lambda^2 \), we find two possible solutions of (1) for \( n_0 \) at the mean field critical temperature, \( n_{mf} = 0 \), 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 \( n_0 \ll t \).

To go beyond mean field we analyze the structure of the self-energies by expanding \( \Sigma_{11} - \Sigma_{11}^{mf} \) and \( \Sigma_{12} - \Sigma_{12}^{mf} \) in a series in \( a \) and the mean field Green’s functions \( G_{11}^{mf} \) and \( G_{12}^{mf} \), given by Eq. (2) with the \( \Sigma_{ij} \) replaced by \( \Sigma_{ij}^{mf} \). We eliminate \( \mu \) in \( \tilde{G} \) 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, \( \xi \), as in [1], defined by

\[
\mu - (\Sigma_{11}^{mf} - \Sigma_{12}^{mf}) = (\Sigma_{11}(0) - \Sigma_{12}(0)) - (\Sigma_{11}^{mf} - \Sigma_{12}^{mf}) = -1/2m\xi^2.
\]

(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, \( \Sigma_{12} \) is formally at least of order \( n_0 \). Diagrams of order \( a^3 \) with \( k \leq 3 \) in the formal expansion contain vertices with two Green’s functions entering; similar to the structure at \( T_c \), they involve the dimensionless combinations \( a\xi/\lambda^2 \) and \( n_0\lambda^2 \xi \). The latter part originates from the dependence of \( G^{mf} \) on \( 2m\Sigma_{12}^{mf} \sim an_0 \). 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 \( 2mT \int d^3 k/(k^2 + \xi^{-2}) \sim \xi^{-1} \lambda^{-2} \), in a loop integral of order \( (a\xi/\lambda^2)^2 \), by \( n_0 \). The explicit \( n_0 \) dependences therefore enter in the combination \( (a\xi/\lambda^2)^2(n_0\lambda^2) = a^2 n_0 \xi^2/\lambda^2 \). Then with all momenta \( k \) scaled by \( 1/\xi \), we find the following scaling structure for the self-energies:

\[
(\Sigma_{ij}(k) - \Sigma_{ij}^{mf}(0)) = T\frac{a^2}{\xi} s \sigma_{ij} \left( \frac{a\xi}{\lambda^2}, n_0\lambda^2 \xi \right).
\]

(9)

where the \( \sigma_{ij} \) are dimensionless functions of dimensionless variables. In particular, for vanishing \( k \),

\[
(\Sigma_{11}(0) - \Sigma_{12}(0)) - (\Sigma_{11}^{mf}(0) - \Sigma_{12}^{mf}(0)) = T\frac{a^2}{\xi} s \left( \frac{a\xi}{\lambda^2}, n_0\lambda^2 \xi \right).
\]

(10)

where \( s \) is a dimensionless function. Equations (8) and (10) imply that

\[
\xi = \frac{\lambda^2}{a} h(n_0\lambda^4/a),
\]

(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 \( a/\lambda^4 \); 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,
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, \( f(x \to 0) \sim x^{-\beta} \), or

\[
\frac{n_0}{n} \sim \left(\frac{a}{\lambda}\right)^{1-\beta} t^{\beta}, \quad t \to a/\lambda,
\]

where \( \beta \) 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 \( t = t_0 = (T_c - T_0)/T_c \sim a \), 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 \( U(k) = 2m(\Sigma_{11}(k) - \Sigma_{11}(0)) \), we have

\[
e_k + \Sigma_{11}(k) - \mu = (k^2 + U(k) + 2m\Sigma_{12})/2m.
\]

Taking for \( \Sigma_{12}(k) \) only the first order diagram in \( n_0 \), we get

\[
\Delta n \approx -\frac{4mgn_0}{\pi \lambda^2} \int_0^\infty dk \frac{k^2}{(k^2 + U(k))(k^2 + U(k) + 4mgn_0)}.
\]

We refer 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],

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

where \( G^{-1}(k) = \mu - e_k - U(k)/2m \) is the inverse of the \((\zeta_n = 0)\) Green’s function at the transition temperature. A free particle 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, \( U(k) \approx k^{1/2}k^{1/2} \), for nonzero \( k \approx k_c \), with \( k_c = (2(2\pi)^{1/2}) \approx 20.7a/\lambda^2 \) [1]. A change of the power-law of the free propagator to \( G(k) \sim k^{-\gamma} \), for \( k \to 0 \), with \( \gamma > 0 \), is possible only at precisely \( T_c \), where the correlation length diverges. As long as \( n_0 \neq 0 \), the Bogoliubov operator inequality [9], \( -G_{11}(k,0) \geq m_{n_0}/n k^2 \), does not permit \( \gamma > 0 \). Therefore the \( z_\eta = 0 \) spectrum remains quadratic, \( \eta = 0 \), as \( k \to 0 \), everywhere below and above the critical temperature.

However, for \( n_0a^4 \ll a \), the details of the spectrum at small \( k \) do not enter, and we may approximate the self-energy as

\[
U(k) = \begin{cases} k_c^{1/2}k^{1/2}, & k \ll k_c, \\ k_c^{1/2}, & k \gg k_c, \end{cases}
\]

which in Eq. (14) leads to

\[
\Delta \bar{n} \approx \begin{cases} (32n_0a/3k_c\lambda^2)\ln(16\pi n_0a/k_c^2): & n_0A^4 \ll a, \\ -(2\pi^{1/2}/\lambda^2)(n_0A^2)^{1/2}: & n_0A^4 \gg a. \end{cases}
\]

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 \( tn_0 \) must be a dimensionless function of the variable \( \lambda^4 n_0/a \). In the limit \( n_0A^4 \ll a \), we may write, using the upper result in Eq. (17),

\[
n_0 + \Delta \bar{n} = \frac{3}{2} n t \approx n_0 \left[ 1 + \frac{32a}{3k_c\lambda^2} \ln \left( \frac{16\pi n_0a}{k_c^2} \right) \right],
\]

where the first term is an expansion of the scaling form

\[
n_t \sim n_0 \left( \frac{\lambda^4 n_0}{a} \right)^{32a/3k_c\lambda^2},
\]

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 \( 2\beta = 1/(1 + (5/6\pi)^{1/2}) = 0.66 \), in excellent agreement with the value \( 2\beta \approx 2/3 \) expected for this universality class. In the other limit, \( n_0A^4 \gg a \), 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, \( \rho_s \), related to \( n_0 \) by Josephson’s sum rule [8–10],

\[
\rho_s = -\lim_{k \to 0} \frac{n_0 m^2}{k^2 G_{11}(k,0)}.
\]

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

\[
\rho_s = n_0 m^2 + 2n_0 m^2 \frac{\partial}{\partial k^2} (\Sigma_{11}(k) - \Sigma_{12}(k))|_{k=0}.
\]

for \( T \ll T_c \). 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:

\[
\frac{\rho_s}{m n} = \frac{a}{\lambda^2} f \left( \frac{t a}{\lambda^2} \right) \sim t \approx a/\lambda,
\]

however, the scaling function \( f_p \) is in general different from the scaling function \( f \). Reference [14] obtained the scaling function for \( \rho_p \) in the dilute limit to order
\[ e = 4 - d, \text{ where } d = 3 \text{ is the spatial dimension. In the mean field limit, } t \gg a/k, \text{ the lowest order self-energies are independent of } k^{2}, \text{ so that from Eq. (21) the superfluid mass density coincides with } n_{0} \text{ to order } a. \text{ Thus } f_{s}(x \to \infty) \sim x. \text{ In the critical region, however, } f_{s}(x \to 0) \sim x^{\gamma}, \text{ where } \gamma \text{ is the critical index for the superfluid mass density. Josephson's scaling relation gives } \gamma = 2\beta - \eta \nu \approx 2/3 \text{ for the critical index of the superfluid mass density, where } \nu \approx 2/3 \text{ is the critical exponent of the correlation length [8]. Since our model calculation above does not include the correct } k \to 0 \text{ limit, to which } \rho_{s} \text{ (but not } n_{0}) \text{ is sensitive, it is therefore not suitable for calculating } \rho_{s} \text{ reliably.}

Let us turn to understanding the behavior of } n_{0} \text{ and } \rho_{s} \text{ in large but finite systems, of linear scale } L. \text{ The condensate density, } n_{0}^{L} = n - \bar{n} L \text{ at } T_{c}, \text{ is nonzero for finite } L \text{ and is found to leading order from}

\[ n = n_{0}^{\infty} - T \int_{0}^{\infty} \frac{d^{3}k}{(2\pi)^{3}} G(k, \zeta) \]

\[ = n_{0}^{L} - T \int_{2\pi/\xi}^{\infty} \frac{d^{3}k}{(2\pi)^{3}} G(k, \zeta), \quad (23) \]

where } G \text{ is the infinite size Green's function. Since at } T_{c}, \text{ } G(k \to 0) = -2mC\zeta^{3}/k^{2} - \eta, \text{ where } C \text{ is constant, and } n_{0}^{\infty} = 0, \text{ we find,}

\[ n_{0}^{L} = \frac{4C}{(1 + \eta)\lambda^{2}L} \left( \frac{2\pi \xi}{L} \right)^{\eta}, \quad (24) \]

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. \text{ With this relation we have}

\[ \frac{N^{1/3} \rho_{s}}{mn} = \frac{2}{(1 + \eta)\lambda^{2}n^{2/3}} = \frac{T_{c}}{T_{c}^{0}} \left( \frac{2}{1 + \eta} \zeta(3/2)^{2/3} \right), \quad (25) \]

where the total particle number is given by } N = nL^{3}. \text{ 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 \text{ of } \eta \text{ is nonzero for an interacting Bose gas, the formal } a \to 0 \text{ limit of Eq. (25) does not, however, agree with the ideal gas value, given by the same formula but with } \eta = 0. \text{ 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} \text{ 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 } \rho_{s} \text{ above and at } T_{c} \text{ follows directly from the definition of the transverse current-current correlation function. Since } G^{-1}(k \to 0) \sim k^{2} \text{ below } T_{c}, \text{ Eq. (20) implies that both Bose condensation and superfluidity set in at the same critical temperature, } T_{c}, \text{ 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 } \rho_{s}, n_{0}, \text{ and } G(k), \text{ as well as derive the Josephson relation from diagrammatic perturbation theory and discuss its relation to transverse current-current correlations.}