Strong-Coupling Bose-Einstein Condensation

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We extend the theory of Bose-Einstein condensation from Bogoliubov’s weak-coupling regime to large s-wave scattering lengths $a_0$. For temperatures below and slightly above the free condensation temperature $T_0$, the model has two phase transitions at $\tilde{\sigma}^1$ and one at $\tilde{\sigma}^2$. At the first, the condensate disappears, at the second, the gas freezes. For zero temperature, $\tilde{\sigma}^2$ lies near the close-packing radius. Our solution satisfies the Nambu-Goldstone theorem, thus avoiding an old problem of many-boson theories.

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1. For $\phi^4$-theory in $D < 4$ Euclidean dimensions with O(N)-symmetry, a powerful strong-coupling theory has been developed in 1998 [1]. It has been carried to 7th order in perturbation theory in $D = 3$ [2], and to 5th order in $D = 4 - \epsilon$ dimensions [3]. The theory is an extension of a variational approach to path integrals set up by R.P. Feynman and collaborator in 1989 [4]. The extension to high orders is called Variational Perturbation Theory (VPT), and is developed in detail in the textbook [2]. Originally, the theory was designed to convert only the divergent perturbation expansions of quantum mechanics into exponentially fast convergent expressions [6]. In the papers [3], it was extended from quantum mechanics to $\phi^4$-theory with its anomalous dimensions and produced all critical exponents. This is called quantum-field-theoretic VPT. That theory is explained in the textbook [2] and a recent review [5].

Surprisingly, this successful theory has not yet been applied to the presently so popular phenomena of Bose-Einstein condensation. These have so far mainly been focused on the semiclassical treatments using the good-old Gross-Pitaevskii equations, or to the weak-coupling theory proposed many years ago by Bogoliubov [10]. This is somewhat surprising since the subject is under intense study by many authors. So far, only the shift of the critical temperature has been calculated to high orders [11]. There are only a few exceptions. For instance, a simple extension of Bogoliubov’s theory to strong couplings was proposed in [13] and pursued further in [14]. But that had an unpleasant feature that it needed two different chemical potentials to maintain the long-wavelength properties of Nambu-Goldstone excitations required by the spontaneously broken U(1)-symmetry in the condensate. For this reason it remained widely unnoticed. Another notable exception is the theory in [15] which came closest to our approach, since it was also based on a variational optimization of the energy. But by following Bogoliubov in identifying $a_0$ as $\sqrt{\rho_0}$ from the outset, they ran into the notorious problem of violating the Nambu-Goldstone theorem. Another approach that comes close to ours is found in the paper [16]. Here the main difference lies in the popular use the Hubbard-Stratonovic transformation (HST) to introduce a fluctuating collective pair field [17]. But, as pointed out in [24] and re-emphasized in [25], this makes it impossible to calculate higher-order corrections [26].

The rules for applying VPT to nonrelativistic quantum field theories in 3+1 dimensions have been specified some time ago [18]. In this note we want to show how derive from them, to lowest order, the properties of the Bose-Einstein condensation at arbitrarily strong couplings.

It must be mentioned that in the literature, there have been many attempts to treat the strong-coupling regime of various field theories for models with a large number of identical field components (the so-called large-N-models). This has first been done for the so-called spherical model [19], later the Gross-Neveu model [20], and O(N)-symmetric $\varphi^2$-models [21]. In all these applications, the leading large-N limit has been easily solved with the help of the HST trick of introducing a fluctuating field variable [22, 23] and a few dominant collective phenomena (Collective Quantum Field Theory [17]). This approach has, however, the above-discussed problems of going to higher orders [25], which are absent here.

2. The Hamiltonian of the boson gas has a free term

$$H_0 \equiv \sum_p a_p^\dagger (\varepsilon_p - \mu) a_p = \sum_p a_p^\dagger \Sigma_p a_p,$$  

(1)

where $\varepsilon_p \equiv p^2/2M$ are the single-particle energies and $\xi_p \equiv \varepsilon_p - \mu$ the relevant energies in a grand-canonical ensemble. As usual, $a_p^\dagger$ and $a_p$ are creation and annihilation operators defined by the canonical equal-time commutators of the local fields $\psi(x) = \sum_p \psi(p/\hbar) a_p$. The local interaction is

$$H_{\text{int}} = \frac{g}{2V} \sum_{p, p', q} a_{p+q}^\dagger a_{p'}^\dagger a_{p'} a_p.$$  

(2)

Instead of following Bogoliubov in treating the $p = 0$ modes of the operators $a_p$ classically and identifying with the square-root of the condensate density $\rho_0$, we introduce the field expectation $\langle \psi \rangle \equiv \sqrt{V \Sigma_0/g}$ as a variational parameter, and rewrite $H_{\text{int}}$ as $H_{\text{int}}^\prime = (V/2g)\Sigma_0^\prime$.
plus
\[ H_{\text{int}}'' = \frac{1}{2} \sum_{p \neq 0} \left[ 2\Sigma_0 \left( a_p^\dagger a_p + a_p^\dagger a_{-p} \right) + \Sigma_0 \left( a_p^\dagger a^\dagger_{-p} + h.c. \right) \right], \] (3)

plus a fluctuating Hamiltonian \( H_{\text{int}}'' \), which looks like (2), except that the sum contains only nonzero-momentum modes. Now we proceed according to the rules of VPT and introduce dummy variational parameters \( \Sigma \) and \( \Delta \) via an auxiliary Hamiltonian
\[ \hat{H}_{\text{trial}} = \frac{1}{2} \sum_{p \neq 0} \left[ \Sigma \left( a_p^\dagger a_p + a_p^\dagger a_{-p} \right) + \Delta a_{-p} a_p + h.c. \right], \] (4)

leading a harmonic Hamiltonian
\[ H_0'' \equiv -\frac{V}{g} \frac{\mu}{\Sigma_0} + \frac{V}{2g} \Sigma_0^2 + \left( \epsilon_p - \mu + 2\Sigma_0 + \Sigma \right) a_p^\dagger a_p \]
\[ + \frac{1}{2} \sum_{p \neq 0} \left( \Sigma_0 + \Delta \right) \left( a_p^\dagger a_p + h.c. \right), \] (5)

for which we have to calculate the energy order by order in perturbation theory considering
\[ H_{\text{int}}^{\text{var}} = H_{\text{int}}'' - \hat{H}_{\text{trial}}. \] (6)

as the interaction Hamiltonian. The zeroth-order variational energy is \( W_0 = \langle H_0'' \rangle \), and the lowest-order correction comes from the expectation value \( \Delta_1 W = \langle H_{\text{var}}' \rangle \). If the energy is calculate to all orders in \( H_{\text{int}}^{\text{var}} \), the result will be independent of the variational parameters \( \Sigma_0, \Sigma, \) and \( \Delta \), but the energy to any finite order will depend on it. The optimal values of the parameters are found by optimization (usually extremization), and the results converge exponentially fast as a function of the order 3. 3. 8.

A Bogoliubov transformation with as yet undetermined coefficients \( u_p, v_p \) constrained by the condition \( u_p^2 - v_p^2 = 1 \), produces a ground state with vacuum expectation values \( \langle a_p a_p \rangle = v_p^2 \) and \( \langle a_p a_{-p} \rangle = u_p v_p \), so that
\[ W_0 = -\frac{V}{g} \frac{\mu}{\Sigma_0} + \frac{V}{2g} \Sigma_0^2 \]
\[ + \sum_{p \neq 0} \left( \epsilon_p - \mu + 2\Sigma_0 + \Sigma \right) v_p^2 + \left( \Sigma_0 + \Delta \right) u_p v_p. \] (7)

The first-order variational energy \( W_1 \) contains, in addition, the expectation value (\( H_{\text{int}}^{\text{var}} \)). Of this, the first part, \( W_{11} = \langle H_{\text{int}}'' \rangle \), is found immediately with the help of the standard commutation rules as a sum of three pair terms
\[ \langle a_{p+q}^\dagger a_{p-1} a_p a_p h.c. \rangle = \langle a_{p+q}^\dagger a_{p-1} a_p a_p h.c. \rangle \]
\[ + \langle a_{p+q}^\dagger a_{p-1} a_p a_p h.c. \rangle + \langle a_{p+q}^\dagger a_{p-1} a_p a_p h.c. \rangle. \] (8)

so that
\[ W_{11} = \langle H_{\text{int}}'' \rangle = \frac{g}{2V} \sum_{p \neq 0} \left( 2v_p^2 u_p^2 + u_p v_p u_p v_p^\dagger \right). \] (9)

The second part \( \langle -\hat{H}_{\text{trial}} \rangle \) adds to this the expectation value
\[ W_{12} = -\sum_{p \neq 0} \left( \Sigma v_p^2 + \Delta u_p v_p \right). \] (10)

In order to fix the average total number of particles \( N \), we differentiate \( W_1 \equiv W_0 + W_{11} + W_{12} \) with respect to \( -\mu \) and set the result equal to \( N \) to find the density \( \rho = N/V \) as
\[ \rho = \frac{\Sigma_0}{g} + \sum_{p \neq 0} v_p^2. \] (11)

The momentum sum is the density of particles outside the condensate, the uncondensed particle density
\[ \rho_u = \sum_{p \neq 0} \langle a_p^\dagger a_p \rangle = \frac{1}{V} \sum_p v_p^2, \] (12)

implying that \( \Sigma_0/g \) is the condensate density \( \rho_0 \):
\[ \frac{\Sigma_0}{g} = \rho_0 = \rho - \rho_u. \] (13)

If we extremize \( W_1 \) with respect to the variational parameter \( \Sigma_0 \), we find the equation
\[ \frac{\mu - \Sigma_0}{g} = \sum_{p \neq 0} (2v_p^2 + u_p v_p) = 2\rho_u + \sum_{p \neq 0} u_p v_p = 2\rho_u + \delta. \] (14)

Let us now determine the size of the Bogoliubov coefficients \( u_p, v_p \). The original way of doing this is algebraic, based on the elimination of the off-diagonal elements of the transformed Hamiltonian operator. In the framework of our variational approach it is more natural to use the equivalent procedure of extremizing the energy expectation \( W_0 \) with respect to \( u_p \) and \( v_p \) under the constraint \( u_p^2 - v_p^2 = 1 \), so that \( \delta u_p/v_p = v_p/u_p \). Doing this, we obtain for each nonzero momentum the equation
\[ 2(\epsilon_p - \mu + 2\Sigma_0 + \Sigma) v_p + (\Sigma_0 + \Delta) (u_p + v_p^2)/u_p = 0. \] (15)

In order to solve this we introduce the constant
\[ \Sigma = -\mu + 2\Sigma_0 + \Sigma = -\mu + 2g(\rho - \rho_u) - \Sigma, \] (16)

the right-hand side emerging after using (12) and (13).

We further introduce the constant
\[ \Delta = \Sigma_0 + \Delta. \] (17)

so that we can rewrite (15) in the simple form
\[ 2(\epsilon_p + \Sigma) v_p + \Delta (u_p + v_p^2)/u_p = 0. \] (18)
which is solved by the Bogoliubov transformation coefficients

\[ u_p^2 = \frac{1}{2} \left( 1 + \frac{\varepsilon_p + \Sigma}{\varepsilon_p} \right), \quad v_p^2 = \frac{1}{2} \left( 1 - \frac{\varepsilon_p + \Sigma}{\varepsilon_p} \right), \tag{19} \]

with \( u_p v_p = \Delta / 2 \varepsilon_p \), and the quasiparticle energies

\[ \varepsilon_p = \sqrt{\left( \varepsilon_p + \Sigma \right)^2 - \Delta^2}, \tag{20} \]

According to the Nambu-Goldstone theorem, these have to vanish linearly for \( p \to 0 \). This forces us to set \( \Delta = \bar{\Sigma} \), or

\[ \Delta = \bar{\Sigma} = \Sigma_0, \tag{21} \]

thus avoiding the main hurdle in previous attempts to go beyond the Bogoliubov theory [13].

Having determined the Bogoliubov coefficients, we calculate the momentum sums in Eqs. (12) and (14). In the lowest approximation, the uncondensed particle density

\[ \rho_a \equiv \frac{1}{V} \sum_p u_p^2 = \frac{1}{2} \int \frac{d^3p}{(2\pi\hbar)^3} \left( \frac{\varepsilon_p + \bar{\Sigma}}{\varepsilon_p} - 1 \right). \tag{22} \]

The integral is easily done if we set \( |p| \equiv \hbar k \kappa \) with \( k = \sqrt{2M\Sigma_0/\hbar} \), so that we find

\[ \rho_a = \frac{k^2}{2} I_{\rho_a}/4\pi^2, \tag{23} \]

where

\[ I_{\rho_a} \equiv \int_0^\infty d\kappa \kappa^2 \left( \frac{\kappa^2 + 1}{\sqrt{(\kappa^2 + 1)^2 - 1}} - 1 \right) = \frac{\sqrt{2}}{3}. \tag{24} \]

The second momentum sum in Eq. (14) reads, after inserting (19):

\[ \delta \equiv \sum_{p \neq 0} (u_p v_p) = \frac{1}{V} \sum_{p \neq 0} u_p v_p = -\frac{\Sigma}{2} \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{\varepsilon_p}. \tag{25} \]

In contrast to (22), this is a divergent quantity. However, as a consequence of the renormalizability of the theory, the divergence can be removed by absorbing it into the inverse coupling constant of the model defined by

\[ \frac{1}{g_R} = 1 + \frac{1}{g} \sum_{p \neq 0} \frac{1}{2\varepsilon_p} = 1 - \frac{1}{g} \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{2\varepsilon_p}. \tag{26} \]

The renormalized coupling is finite and measurable in two-body scattering as an s-wave scattering length: \( g_R = 4\pi\hbar^2 a_{\rho}/M \). Thus we introduce the finite renormalized quantity

\[ \delta_R = \frac{1}{V} \sum_p u_p v_p = -\frac{\Sigma}{2} \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{\varepsilon_p} - \frac{1}{2\varepsilon_p}. \tag{27} \]

and write \( \delta = \delta_R + \delta_{\text{div}} \), where the divergence is the momentum sum

\[ \delta_{\text{div}} \equiv -\frac{\bar{\Sigma}}{V} \sum_p \frac{1}{(2\varepsilon_p)} = -\frac{\bar{\Sigma}}{2} \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{2\varepsilon_p}. \tag{28} \]

If we denote this by \(-\bar{\Sigma}/Vv\), we have

\[ \delta = \delta_R + \delta_{\text{div}} = \delta_R - \frac{\bar{\Sigma}}{Vv}. \tag{29} \]

Inserting this together with (12) into (14), we find

\[ \frac{\mu - \Sigma_0}{g} = 2\rho_a + \delta_R + \delta_{\text{div}}. \tag{30} \]

Recalling (13), this implies

\[ \frac{\mu}{g} = \rho_0 + 2\rho_a + \delta_R + \delta_{\text{div}} = \rho + \rho_a + \delta_R + \delta_{\text{div}}. \tag{31} \]

If we evaluate the momentum sum \( 2\bar{\Sigma} \) by the same procedure as in (22), it yields

\[ \delta_R = k_0^2 I_\delta/4\pi^2, \tag{32} \]

where \( I_\delta \) is given by the integral

\[ I_\delta \equiv -\int_0^\infty d\kappa \kappa^2 \left( \frac{1}{\sqrt{(\kappa^2 + 1)^2 - 1}} - \frac{1}{\kappa^2} \right) = \sqrt{2}. \tag{33} \]

We observe that

\[ I_\delta = 3I_{\rho_a}. \tag{34} \]

We continue the discussion by rewriting Eq. (10), with the help of (31), as

\[ \frac{\bar{\Sigma}}{g} = \rho - 3\rho_a - \delta_R - \frac{\bar{\Sigma}}{Vv}. \tag{35} \]

As before in Eqs. (26), (28), and (29), the last, divergent term can be absorbed into the first by renormalizing the coupling constant, so that we obtain

\[ \frac{\bar{\Sigma}}{g} = \frac{\bar{\Sigma}}{g_R} + \rho - 3\rho_a - \delta_R. \tag{36} \]

Similarly we can use Eq. (21) to see that

\[ \frac{\Delta}{g} = \frac{\bar{\Sigma}}{g_R} - \rho + \rho_a. \tag{37} \]

Finally, we calculate the total variational energy \( W_1 \). Inserting the Bogoliubov coefficients (13) into \( W_0 \) of Eq. (7), and adding the energies \( W_{11} + W_{12} \) of and (9) and (10), we have

\[ W_1 = -\frac{V}{2g} \rho \Sigma_0 + \frac{V}{2g} \Sigma_0^2 + Vw(\bar{\Sigma}) - \frac{\Sigma_0^2}{4Vv} + W_{11} + W_{12}, \tag{38} \]
where $w(\bar{\Sigma})$ is the convergent momentum sum

$$w(\bar{\Sigma}) \equiv \frac{1}{2V} \sum_{\nu \neq 0} \left\{ \varepsilon_{\nu} - \varepsilon_{\nu} - \bar{\Sigma} + \frac{\varepsilon_{\nu}^2}{2\varepsilon_{\nu}} \right\}. \quad (39)$$

This is evaluated as in (22) to be

$$w(\bar{\Sigma}) = \Sigma k_0^2 I_E/4\pi^2, \quad (40)$$

where

$$I_E \equiv \int_0^\infty d\kappa^2 \left[ \sqrt{(\kappa^2+1)^2-1} - \kappa^2 - 1 + \frac{1}{2\kappa^2} \right]. \quad (41)$$

If we rename all $I/4\pi^2$'s to $\bar{I}$'s, the energy $W_1$ becomes

$$W_1 = \frac{V}{g} \sum_{\nu \neq 0} \left\{ \frac{V}{2g} \Sigma_0 + V \Sigma k_0^2 I_E \right\} + \frac{V}{g} \sum_{\nu \neq 0} \left\{ \frac{V}{2g} \Sigma k_0^2 I_E \right\} \quad (42)$$

$$+ \frac{V}{g^2} \sum_{\nu \neq 0} \left\{ 2I_\nu^2 + I_\delta^2 \right\} - V \Sigma k_0^2 (\Sigma I_{\rho a} + \Delta I_\delta).$$

The expression is renormalized via dimensional regularization, which allows us to use Veltman’s rule [7] to set $1/\nu = 0$.

We are now prepared to extremize the variational energy Eq. (12) with respect to $\bar{\Sigma}$. We insert $-\Sigma/g \equiv \rho - 3\rho_a - \delta_R - \Sigma/g$ from (36) and $-\Delta/g \equiv \rho - \rho_a - \Sigma/g$ from (17) and vary $W_1$ in $\delta\Sigma$ to find

$$\left( \frac{\Sigma}{g} - \rho(\nu) \right)' + \left( \frac{\Sigma}{g} - \rho(\nu) \right) = 0, \quad (43)$$

where $\rho(\nu) \equiv \rho - \rho_a \pm \delta_R$. This equation is solved by

$$\frac{\Sigma}{g} = \rho - \rho_a - \delta_R \frac{\rho(\nu)'}{\rho(\nu) + \delta}, \quad (44)$$

Using the zero-temperature relation $I_\delta = 3I_{\rho a}$ from (34), this becomes

$$\frac{\Sigma}{g} = \rho + \frac{1}{2} \rho(\nu). \quad (45)$$

3. To extract experimental consequences it is useful to re-express all equations in a dimensionless form by introducing the reduced variables

$$s \equiv \frac{\Sigma}{\epsilon_a}, \quad (46)$$

where $\epsilon_a \equiv \hbar^2/2Ma^2$ is the natural energy scale of the system. We also introduce the reduced $s$-wave scattering length

$$\hat{a}_s \equiv \frac{8\pi a_s}{a}, \quad (47)$$

in terms of which the renormalized coupling constant is

$$g_R = \frac{4\pi\hbar^2}{M} a_s = 8\pi\epsilon_a a^2 a_s = \epsilon_a a^2 \hat{a}_s, \quad (48)$$

while

$$k_\Sigma = \sqrt{s}, \quad \frac{\Sigma}{g_R} = \frac{s}{8\pi a^2 a_s} = \frac{s}{3a^2 a_s}, \quad (49)$$

and the sound velocity reads

$$c = \sqrt{\frac{3}{2} v_a}, \quad v_a \equiv \frac{p_a}{M} = \frac{\hbar}{aM}. \quad (50)$$

Let us also define the reduced quantities

$$\bar{\rho}_a \equiv \rho_\nu/\rho = s^{3/2} I_{\rho a}, \quad \bar{\rho} \equiv \delta/\rho = s^{3/2} I_\delta. \quad (51)$$

The relation between $s$ and $\hat{a}_s$ is from (48) and (18):

$$\frac{s}{\hat{a}_s} = 1 + \frac{1}{2} s^{3/2} I_{\rho a} = 1 + \frac{\sqrt{2}}{24\pi^2} s^{3/2}. \quad (52)$$

It is plotted in Fig. (1b). The corresponding behavior of $\bar{\rho}_{\rho a}$ is shown in Fig. (1c).

Using of $\bar{\rho}_a$ and $\bar{\rho}$ from (51), we calculate from Eq. (12) the reduced variational energy $w_1 \equiv W_1/N\epsilon_a$. We go from the grand-canonical to the proper energies by adding $\mu N$ to $W_1$ and forming $W^c = W_1 + \mu V \rho$. In this way we obtain the reduced energy density per particle

$$w_1^c = \frac{\hat{a}_s}{2} + \frac{\sqrt{2}}{3\pi^2} \hat{a}_s^{3/2} - \frac{\sqrt{2}}{3\pi^2} \hat{a}_s^{3/2} + \frac{\hat{a}_s}{72\pi^4} s^{3/2}. \quad (53)$$

Inserting (52), we find that up to the term $\hat{a}_s^4$ the expansion

$$w_1^c = \frac{\hat{a}_s}{2} + \frac{\sqrt{2}}{15\pi^2} \hat{a}_s^{3/2} + \frac{1}{72\pi^4} \hat{a}_s^4 + \ldots. \quad (54)$$

In Fig. (2) we compare the reduced total energy $w_1^c$ with Bogoliubov’s result

$$w_1^{\text{Bog}} = \frac{\hat{a}_s}{2} + \frac{\sqrt{2}}{15\pi^2} \hat{a}_s^{3/2}. \quad (55)$$

Note that the energy has a singularity at $(\hat{a}_s, s_c) = (16.08, 48.23)$ where the condensate disappears in a continuous phase transition.
There is no problem to increase the accuracy to any desired level, with exponentially fast convergence, as was demonstrated by the calculation of critical exponents in all Euclidean $\varphi^4$ theories with $N$ components in $D$ dimensions [7]. The procedural rules were explained in the paper [22]. We merely have to calculate higher-order diagrams using the harmonic Hamiltonian [11] as the free action, and [21] as the interaction Hamiltonian that determines the vertices. At any given order, the results are optimized in the variational parameters $\Sigma_0$, $\Sigma$, and $\Delta$. The theory is renormalizable, so that all divergencies can be absorbed in a redefinition of the parameters of the original action, order by order. This is the essential advantage of the present theory over any previous strong-coupling scheme published so far in the literature, in particular over those based on Hubbard-Stratonovic transformations of the interaction, which are applicable only in some large-$N$ limits [20]. The second diagram in Eq. (3.741) of the textbook [5]. Its contribution would be the $3+1$-dimensional version of the last term in Eq. (3.767), is essential in the $X \neq 0$ phase. Without this term, the slope of the quantum-mechanical energy as a function of the coupling constant is missed by 25%, as discussed in the heading of Fig. 5.24.

1 The second diagram in Eq. (3.741) of the textbook [5]. Its contribution would be the $3+1$-dimensional version of the last term in Eq. (3.767), is essential in the $X \neq 0$ phase. Without this term, the slope of the quantum-mechanical energy as a function of the coupling constant is missed by 25%, as discussed in the heading of Fig. 5.24.

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\[ \tilde{\alpha}_s = 8\pi a_s/a \]

\[ w_s^\dagger = W_1/N\varepsilon_a \]

\[ W_{\text{Bog}} \]

\[ \tilde{\alpha}_s \approx 8\pi a_s/a \]

\[ w_s^\dagger = W_1/N\varepsilon_a \]

\[ \text{compared with Bogoliubov's weak-coupling result} \text{. There is a continuous phase transition at} (\tilde{\alpha}_s, s) \approx (16.08, 48.23), \text{where the condensate becomes depleted and the ratio} \rho_{\text{at}}/\rho \text{reaches unity.} \]


