

# On the Bose–Einstein condensation temperature in a trap

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**Abstract.** A mean-field semiclassical approach to the calculation of the transition temperature for an interacting Bose gas in a trap is presented. The interaction changes the dependence of the condensation temperature on the number of particles.

**Keywords:** Bose Einstein condensation (theory), critical exponents and amplitudes (theory), quantum many body problems

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**1. Introduction**

I experience pleasure mixed with melancholy writing this paper honoring the 60th birthday of Thomas Nattermann. Our first meeting took place in the German Democratic Republic in the 1970s, when Thomas was a very young faculty member at the University of Leipzig. During the 30 years or so of our friendship I have admired Thomas' scientific and personal integrity; I have benefited a lot from his clear understanding of physics of disordered systems and I deeply respect his fundamental contribution to this field of physics. But no less do I admire his attitude to physics as a whole, and his desire to include what he is doing in a general frame. Communication with Thomas is always rewarding, not only because he is a clever and interesting physicist, but also due to his charisma and invariant kindness. I wish him many years of fruitful work and happy life with his family.

In this paper I calculate the condensation temperature of an interacting Bose gas confined in a harmonic trap. This problem was solved long ago for a non-interacting Bose gas. I show how to do it for an interacting Bose gas. This work is preparation for a more interesting problem about the influence of the disorder on the Bose–Einstein condensation temperature which we discussed recently with Thomas. Though mathematic difficulties still preclude the advance of this project, I decided to publish the part related to a completely ordered trap separately, since the results are new and seem interesting.

**2. General approach**

We start with the self-consistent equation for the density  $n(\mathbf{r})$  above the phase transition. The idea is that the size of the trap is much larger than the thermal de Broglie wavelength  $\hbar/\sqrt{2mT}$ . Then the momentum and the coordinate are defined simultaneously with good precision. One can introduce the Bose–Einstein occupation numbers at a given point in the space:

$$n(\mathbf{p}, \mathbf{r}) = \left[ \exp \left( \frac{\mathbf{p}^2/2m + U(\mathbf{r}) - \mu}{T} \right) - 1 \right]^{-1}, \quad (1)$$

where  $\mu$  is the chemical potential and  $U(\mathbf{r})$  is the self-consistent field. It can be expressed as the sum of the trap field  $V(\mathbf{r})$  and the self-interaction field  $gn(\mathbf{r})$ , where  $g$  is the interaction constant, associated with the scattering length  $a$  by the standard relation  $g = 4\pi\hbar^2 a/m$ , and  $n(\mathbf{r})$  is the density of bosons at the point  $\mathbf{r}$ :

$$U(\mathbf{r}) = V(\mathbf{r}) + gn(\mathbf{r}). \quad (2)$$

The self-consistent equation for the particle density at a given point reads

$$n(\mathbf{r}) = \int n(\mathbf{p}, \mathbf{r}) \frac{d^3p}{(2\pi\hbar)^3}. \quad (3)$$

The equation for chemical potential with a fixed number of particles  $N$  reads

$$\int n(\mathbf{r}) d^3x = \int \frac{d^3p d^3x}{(2\pi\hbar)^3} \left[ \exp\left(\frac{\mathbf{p}^2/2m + U(\mathbf{r}) - \mu}{T}\right) - 1 \right]^{-1} = N. \quad (4)$$

Since the occupation numbers must be positive, the chemical potential obeys the inequality  $\mu \leq U_{\min}$ . At the Bose–Einstein condensation temperature the occupation number becomes infinite at  $\mathbf{p} = 0$  and at the point in space in which the self-consistent potential reaches its minimum value  $U_{\min}$ . Thus, the transition temperature is determined by the equation

$$\int \frac{d^3p d^3x}{(2\pi\hbar)^3} \left[ \exp\left(\frac{\mathbf{p}^2/2m + U(\mathbf{r}) - U_{\min}}{T_c}\right) - 1 \right]^{-1} = N \quad (5)$$

together with equations (2) and (3). It is convenient to introduce  $W(\mathbf{r}) = U(\mathbf{r}) - U_{\min}$  and rewrite equations (2) and (3) for the density in the transition point as follows:

$$W(\mathbf{r}) = V(\mathbf{r}) - V^* + g \int \frac{d^3p}{(2\pi\hbar)^3} \times \left\{ \left[ \exp\left(\frac{\mathbf{p}^2/2m + W(\mathbf{r})}{T_c}\right) - 1 \right]^{-1} - \left( \exp\frac{\mathbf{p}^2}{2mT_c} - 1 \right)^{-1} \right\}, \quad (6)$$

where  $V^*$  is the value of  $V(\mathbf{r})$  at the minimum of  $U(\mathbf{r})$ , or equivalently, at the node of  $W(\mathbf{r})$ . In these terms, equation (5) also is simplified:

$$\int \frac{d^3p d^3x}{(2\pi\hbar)^3} \left[ \exp\left(\frac{\mathbf{p}^2/2m + W(\mathbf{r})}{T_c}\right) - 1 \right]^{-1} = N. \quad (7)$$

### 3. Non-interacting gas in a harmonic trap

For illustration we consider a well-known and already solved problem of a non-interacting gas of bosons in a harmonic trap [1]. The standard solution uses the 3D oscillator energy levels  $\varepsilon_{n_1, n_2, n_3} = \hbar[(n_1 + \frac{1}{2})\omega_1 + (n_2 + \frac{1}{2})\omega_2 + (n_3 + \frac{1}{2})\omega_3]$  and calculates the total number of particles at  $T = T_c$  and  $\mu = (\hbar/2)(\omega_1 + \omega_2 + \omega_3)$ :

$$\sum_{n_1, n_2, n_3=0}^{\infty} \left[ \exp\frac{\hbar(n_1\omega_1 + n_2\omega_2 + n_3\omega_3)}{T_c} - 1 \right]^{-1} = N. \quad (8)$$

Assuming that  $\hbar\omega_i \ll T_c$ , one can substitute the sum in equation (8) by an integral. After a simple change of variables we arrive at the result:

$$\int_0^\infty \int_0^\infty \int_0^\infty \left[ \exp \frac{\hbar(n_1\omega_1 + n_2\omega_2 + n_3\omega_3)}{T_c} - 1 \right]^{-1} dn_1 dn_2 dn_3 = \left( \frac{T_c}{\hbar\bar{\omega}} \right)^3 \zeta(3), \quad (9)$$

where  $\bar{\omega} = (\omega_1\omega_2\omega_3)^{1/3}$ . From this result and equation (8) there follows the well-known result:  $T_c = \hbar\bar{\omega}(N/\zeta(3))^{1/3}$ . We will rederive this result by integration in the phase space. Employing equation (7) with  $W(\mathbf{r}) = V(\mathbf{r}) = (m/2)(\omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_3^2 x_3^2)$  and changing the variables  $\mathbf{p}, \mathbf{x}$  by  $\mathbf{u} = \mathbf{p}/\sqrt{2mT}$  and  $v_i = \sqrt{(m\omega_i^2/2T)}x_i$  ( $i = 1, 2, 3$ ), we arrive at the following equation:

$$\left( \frac{T_c}{\pi\hbar} \right)^3 \frac{1}{\omega_1\omega_2\omega_3} \int [\exp(\mathbf{u}^2 + \mathbf{v}^2) - 1]^{-1} d^3u d^3v = N. \quad (10)$$

Let us introduce the six-component vector  $\mathbf{w} = (\mathbf{u}, \mathbf{v})$  and a spherical frame of reference in the  $\mathbf{w}$ -space:  $\mathbf{w}^2 = \mathbf{u}^2 + \mathbf{v}^2$ . Then integral in equation (10) can be rewritten as follows:

$$S_5 \int_0^\infty (\exp w^2 - 1)^{-1} w^5 dw, \quad (11)$$

where  $S_5 = \pi^3$  is the surface area of the unit five-dimensional sphere embedded into six-dimensional space. By the next change of variable  $t = w^2$  this integral is reduced to

$$\int_0^\infty (\exp w^2 - 1)^{-1} w^5 dw = \frac{1}{2} \int_0^\infty t^2 (e^t - 1)^{-1} dt = \zeta(3). \quad (12)$$

Combining equations (10)–(12), we arrive at the same value for the transition temperature:

$$T_c = \hbar\bar{\omega}(N/\zeta(3))^{1/3}. \quad (13)$$

#### 4. Interacting gas in a harmonic trap

In this section we consider a spherically symmetric trap for simplification of the formulae ( $\omega_1 = \omega_2 = \omega_3 = \omega$ ). The generalization to an asymmetric harmonic trap is straightforward. Spherical symmetry of the problem ensures that the function  $U(r)$  has either a minimum or maximum at the origin  $r = 0$ . We assume that it is a minimum. This assumption will be confirmed by direct calculation. According to this assumption,  $W(r) = U(r) - U(0)$ . Thus, equation (6) can be simplified by omitting the term  $V^*$ . We introduce dimensionless variables  $\mathbf{q} = \mathbf{p}/\sqrt{2mT_c}$ ,  $\boldsymbol{\rho} = \sqrt{(m\omega^2/2T_c)}\mathbf{r}$  and  $w = W/T_c$ . In terms of these variables, equation (6) can be rewritten as follows:

$$w = \rho^2 - \gamma f(w), \quad (14)$$

where the function  $f(w)$  is given by an integral:

$$f(w) = \int_0^\infty \left[ \frac{1}{e^x - 1} - \frac{1}{e^{x+w} - 1} \right] \sqrt{x} dx, \quad (15)$$

and the dimensionless coupling constant  $\gamma$  reads

$$\gamma = \frac{gm^{3/2}T_c^{1/2}}{\sqrt{2}\pi^2\hbar^3}. \quad (16)$$

For specific calculations the representation of the function  $f(w)$  by a series is convenient:

$$f(w) = \frac{\sqrt{\pi}}{2} \sum_{n=1}^{\infty} \frac{1 - e^{-nw}}{n^{3/2}}. \quad (17)$$

From the series representation it is easy to extract the asymptotics:

$$f(w) \approx \begin{cases} \pi\sqrt{w}; & w \ll 1 \\ \frac{\sqrt{\pi}\zeta(3/2)}{2} \approx 2.309; & w \gg 1. \end{cases} \quad (18)$$

The graph of the function  $f(w)$  is represented in figure 1. The asymptotic at small  $w$  is extracted from the series representation (17) by the transition from summation to integration (see details in the appendix). From this asymptotic it follows that at small enough  $\rho$  the function  $w$  behaves as  $w \approx \rho^4/(\pi^2\gamma^2)$ , whereas at big enough  $\rho$  the asymptotic of  $w$  reads  $w \approx \rho^2$ . The first asymptotic implies that, at small  $r$ , the density obeys the following asymptotic relation:

$$n(r) = n(0) - \frac{m\omega^2 r^2}{2g} + \frac{m^2\omega^2 r^4}{4\pi^2 T_c g} + O(r^6). \quad (19)$$

It is also interesting that the density at  $r = 0$  does not depend either on the oscillator frequency of the trap or on the interaction constant:

$$n(0) = \zeta\left(\frac{3}{2}\right) \left(\frac{mT_c}{2\pi\hbar^2}\right)^{3/2}. \quad (20)$$

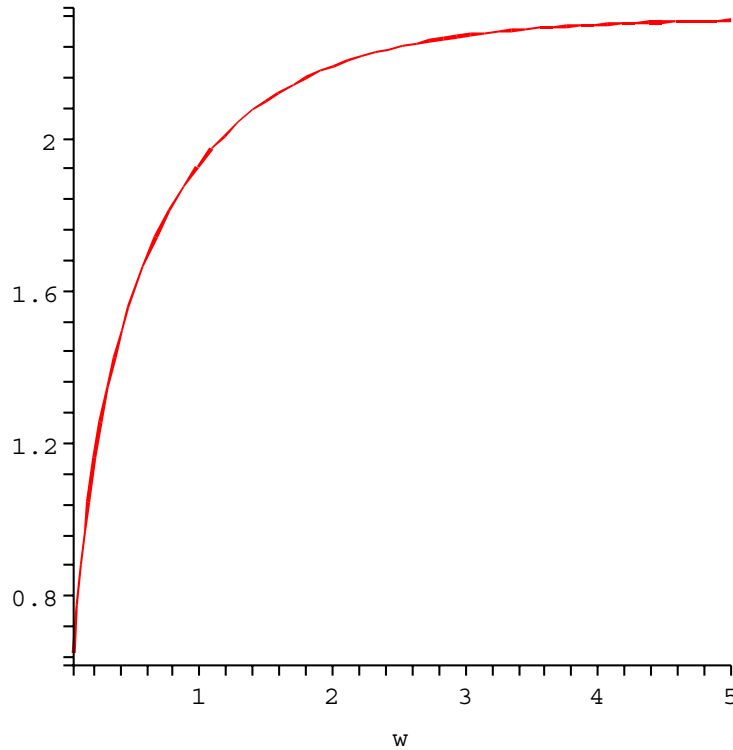
This is the same as for an ideal homogeneous Bose gas with the same critical temperature. Let us analyze the conditions at which the approximate equation (19) and preceding approximate expression for  $w$  versus  $\rho$  are valid. They are based on the asymptotics of the function  $f(w)$  at small  $w$  (first line in equation (18)). It is valid at  $w \ll 1$ , or equivalently, at  $\rho \ll \min(\pi\gamma, \sqrt{\pi\gamma})$ . In standard units this condition reads  $r \ll \min(L_g(T_c/\hbar\omega), (L_g l_{\text{osc}})^{1/2}(T_c/\hbar\omega)^{3/4})$ , where  $L_g = (gm/\pi\hbar^2)$  and  $l_{\text{osc}} = \sqrt{\hbar/m\omega}$ . Employing equations (20) and (16), one can see that the latter inequality ensures that the quadratic in  $r$  correction to the density in equation (19) is much less than  $n(0)$ . The ratio of the next correction proportional to the  $r^4$  to the quadratic one with precision of numerical coefficient is equal to  $W(r)/T_c = w \ll 1$ .

The equation for critical temperature reads as follows:

$$N = \left(\frac{T_c}{\hbar\omega}\right)^3 \frac{4}{\pi} g(\gamma), \quad (21)$$

where

$$g(\gamma) = \int_0^\infty \int_0^\infty dx dy \sqrt{xy} [\exp(x + w(y)) - 1]^{-1} \quad (22)$$



**Figure 1.** Graph of the function  $f(w)$ .

and  $w(y)$  is determined by equation (14) with  $\rho^2 = y$ . By the change of variable  $y$  to  $w$  the function  $g(\gamma)$  is transformed into the following form:

$$g(\gamma) = \int_0^\infty \int_0^\infty dx dw (1 + \gamma f'(w)) \sqrt{x(w + \gamma f(w))} [\exp(x + w) - 1]^{-1}. \quad (23)$$

The series representation is usually more practical:

$$g(\gamma) = \frac{\pi}{\sqrt{3}} \sum_{n=1}^\infty n^{-1/2} \int_0^\infty [w + \gamma f(w)]^{3/2} e^{-nw} dw. \quad (24)$$

We analyze equation (23) in two limiting cases: small and large  $\gamma$ . In the case of small  $\gamma$  the terms containing  $f(w)$  and  $f'(w)$  vanish in the leading approximation, and we arrive at  $g(0) = (\pi/4)\zeta(3)$ . The first-order correction to  $g(\gamma)$  reads

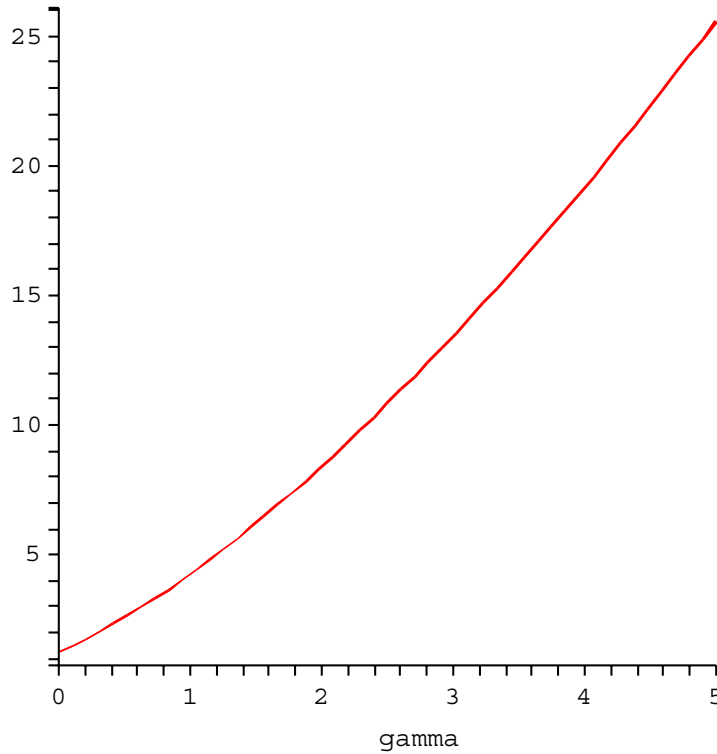
$$\delta_1 g = \gamma \int_0^\infty \int_0^\infty dx dw \sqrt{xw} \left( f'(w) + \frac{f(w)}{2w} \right) [\exp(x + w) - 1]^{-1}. \quad (25)$$

Thus, the corrected value of  $T_c$  reads

$$T_c = T_{c0} \left( 1 - \frac{4C}{\pi\zeta(3)} \gamma_0 \right), \quad (26)$$

where  $T_{c0}$  is the transition temperature for a non-interacting Bose gas determined by equation (13), the constant  $C \approx 3.964$  is equal to the integral in equation (25), and  $\gamma_0$  is the value of  $\gamma$  defined by equation (16) at  $T_c = T_{c0}$ .

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**Figure 2.** Graph of the function  $g(\gamma)$ .

At large  $\gamma$  it is possible to neglect 1 in comparison to  $\gamma f'(w)$  and  $w$  in comparison to  $\gamma f(w)$  in equation (23) and get the following asymptotics for  $g(\gamma)$ :

$$g(\gamma) \approx D\gamma^{3/2}, \tag{27}$$

where the constant  $D \approx 1.873$  is determined by the integral

$$D = \int_0^\infty \int_0^\infty dx dw \sqrt{x} f'(w) \sqrt{f(w)} [\exp(x+w) - 1]^{-1} \tag{28}$$

or the series of integrals

$$D = \frac{\sqrt{\pi}}{3} \sum_{n=1}^\infty n^{-1/2} \int_0^\infty [f(w)]^{3/2} e^{-nw} dw. \tag{29}$$

The graph of the function  $g(\gamma)$  is shown in figure 2. Substituting (28) into the equation for the critical temperature (21) and employing the definition of  $\gamma$  (16), we arrive at the following expression for the transition temperature, valid for a large number of particles or for large coupling constant:

$$T_c = \frac{\pi^{16/15} N^{4/15}}{2^{1/3} D^{4/15}} \frac{\hbar^2 \omega^{4/5}}{m^{3/5} g^{2/5}} = \frac{\pi^{2/3} \hbar \omega N^{4/15}}{2^{17/15} D^{4/15}} \left( \frac{\ell}{a} \right)^{2/5}. \tag{30}$$

Here  $l = \sqrt{\hbar/m\omega}$  is the oscillator length and  $a$  is the scattering length. The dependence of  $T_c$  on  $N$  differs a little from that for a non-interacting gas (the exponent is 4/15 instead

of  $1/3$ ). To satisfy the inequality  $\gamma \gg 1$  the number of particles must obey an inequality:

$$N \gg (2^{15/2} \pi^{5/2} D)^{-1} \left( \frac{\ell}{a} \right)^6. \quad (31)$$

Though the self-consistent approach is not exact, it probably becomes asymptotically exact at small and large gas factor  $na^3$ . Indeed, it is exact at weak interaction to the first approximation in  $g$ . Strong interaction corresponds to  $n^{1/3}a \gg 1$ . This means that a large number  $na^3$  of particles interact with one. The self-consistent field only weakly fluctuates. We did not take into account the renormalization of the mass, but the renormalization factor is not large even at strong interaction. A convincing example is liquid  ${}^4\text{He}$ , whose superfluid transition point can be reasonably estimated by a standard equation for the transition point in an ideal gas with the mass of the helium atom.

The comparison of the equations for the transition temperature of the ideal (13) and strongly interacting (30) gases shows that the dependence on the number of particles differs rather insignificantly (the exponent is  $4/15$  instead of  $1/3$ ), but the transition temperature of the strongly interacting gas contains a factor  $a^{-2/5}$ , which can be regulated by an external magnetic field near the Feshbach resonances [2]. Theory predicts resonance suppression of the condensation temperature near the resonance.

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### Appendix

A simple idea beyond the asymptotics of the function  $f(w)$  at small  $w$  (the upper line in equation (18)) is that the summand  $(1 - \exp(-nw))/n^{3/2}$  in an essential region of summation  $n \lesssim 1/w$  is a slowly varying function of  $w$ . Therefore, the summation in this equation can be replaced by integration:

$$\sum_{n=1}^{\infty} \frac{1 - e^{-nw}}{n^{3/2}} \approx \int_0^{\infty} \frac{1 - e^{-xw}}{x^{3/2}} dx = 2\sqrt{\pi w} \quad (A.1)$$

from which the asymptotic  $f(w) \simeq \pi\sqrt{w}$  immediately follows. It is more difficult to estimate the precision of this approximation. The difference between the sum in equation (17) and integral (A.1) is

$$\Delta = \sum_{n=1}^{\infty} \int_{n-1/2}^{n+1/2} [q(n) - q(x)] dx - \int_0^{1/2} q(x) dx, \quad (A.2)$$

where  $q(x) = (1 - \exp(-wx))/x^{3/2}$ . The last term in (A.2) is easily estimated as  $-\sqrt{2}w$ . Its modulus is much less than the integral (A.1).

In order to estimate the sum in equation (A.2) let us introduce some integer value  $n_1$  such that  $1 \ll n_1 \ll w^{-1}$  and first perform summation over  $n$  from 1 to  $n_1$ . In this region the product  $wn$  is small and one can replace  $q(n) - q(x)$  by  $w[n^{-1/2} - x^{-1/2}]$ . The



integration over  $x$  can be performed explicitly. The sum from 1 to  $n_1$  gives a contribution to  $\Delta$  which we denote  $\Delta_1$ :

$$\Delta_1 = w \sum_{n=1}^{n_1} \left[ n^{-1/2} - 2 \left( n + \frac{1}{2} \right)^{1/2} + 2 \left( n - \frac{1}{2} \right)^{1/2} \right]. \quad (\text{A.3})$$

The series is convergent. Therefore, with a small relative error it is possible to extend the summation in (A.3) to infinity. The result reads  $\Delta_1 \approx -0.046w$ . In the remaining sum from  $n_1$  to  $\infty$  all  $n$  are large and  $x$  in each integral varies between  $-1/2$  and  $+1/2$ . Therefore, with high precision one finds  $q(n) - q(x) \approx -q'(n)(x - n) - \frac{1}{2}q''(n)(x - n)^2$ . After integration over  $x$  from  $n - 1/2$  to  $n + 1/2$  the first term vanishes, whereas the second term gives  $-(q''(n))/24$ . Thus, the sum of these terms from  $n_1$  to  $\infty$  is equal to  $\Delta_2 = -\frac{1}{24} \sum_{n=n_1}^{\infty} q''(n)$ . This sum can be replaced again by an integral with the result  $\Delta_2 = -\frac{1}{24}q'(n_1) = w/48n_1^{3/2} \ll w$ . Thus,  $\Delta_2$  is much less than  $\Delta_1$  at small  $w$ . On the other hand, both corrections to the result (A1) are linear in  $w$  and can be neglected in comparison to the dominant contribution proportional to  $\sqrt{w}$  at small  $w$ .

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