A more accurate analysis of Bose-Einstein condensation in harmonic traps

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Abstract: Using the Euler-Maclaurin summation we calculate analytically the internal energy for non-interacting bosons confined within a harmonic oscillator potential. The specific heat shows a sharp \( \lambda \)-like peak indicating a condensation into the ground state at a well-defined transition temperature. Full agreement is obtained with direct numerical calculation of the same quantities. When the number of trapped particles is very large and at temperatures near and above the transition temperature, the results also agree with previous approximate calculations. At extremely low temperatures both the specific heat and the number of particles excited from the condensate are exponentially suppressed.

Bose-Einstein condensation has now been experimentally demonstrated in magnetic traps of rubidium\(^1\), lithium\(^2\) and most recently sodium\(^3\) gases. To a good approximation one describes the trapping potentials as 3-dimensional anisotropic oscillators which in the rubidium experiments\(^1\) have frequencies typically around \( \omega = 500 - 1000 \) Hz. For the sake of simplification we will here ignore the anisotropy and the weak interactions between the alkali gas atoms. The energy levels of one particle are then simply given as \( \varepsilon_n = \hbar \omega n \) where the quantum number \( n \) takes the values \( n = 0, 1, 2 \ldots \) when we drop the zero-point energy. Since each energy level has a degeneracy \( g_n = (n+1)(n+2)/2 \), the total number \( N \) of particles in such a trap at temperature \( T \) and chemical potential \( \mu \) is given by the Bose-Einstein distribution as

\[
N = \sum_{n=0}^{\infty} \frac{g_n}{e^\beta(\varepsilon_n-\mu) - 1}
\]

where \( \beta = 1/k_B T \). The ground state has quantum number \( n = 0 \) and thus contains \( N_0 = \lambda/(1-\lambda) \) particles where \( \lambda = \exp (\beta \mu) \) is the fugacity. We then have

\[
N = \frac{\lambda}{1-\lambda} + N_e
\]

where the number of particles in the higher states is

\[
N_e = \sum_{n=1}^{\infty} \frac{g_n \lambda e^{-bn}}{1 - \lambda e^{-bn}}
\]
It depends only on the effective fugacity \( \lambda = \lambda \exp (-b) \) where \( b = h\omega/k_BT \).

When the temperature is lowered, the fugacity \( \lambda \to 1 \) and a finite fraction of particles starts to condense into the ground state. Since the total number of particles \( N \gg 1 \), this will happen when the variable \( b \ll 1 \). In this region and at higher temperatures one can then approximate the sum in (3) by an integral. Including only the leading term \( \sim n^2 \) in the degeneracy, one then has the semiclassical limit [4][5]. Defining the transition temperature to be the temperature at which the fugacity takes the value \( \lambda = 1 \), it is then found [4] to be given by

\[
T_0 = \frac{h\omega}{k_B} \left( \frac{N}{\zeta(3)} \right)^{1/3}
\] (4)

The resulting specific heat exhibits a sharp jump with the shape of a \( \lambda \). This is in contrast with the gas in zero potential where the specific heat is continuous. As a check, the partition function was also calculated using numerical summation.

A more accurate approximation of the sum has been given by Grossmann and Holthaus [6]. Based upon the two leading terms in the degeneracy, they constructed a continuous density of states which then made it possible to approximate the sum by two integrals. This caused a small shift in the transition temperature by a factor \( \sim N^{-1/3} \) [4] and a corresponding small rounding-off of the sharp peak in the specific heat when the particle number \( N \) is not too large. In the experiments under consideration, \( N \) takes typically values in the range from \( 10^3 \) to \( 10^6 \).

Recently, these approximation methods in which the sum is replaced by integrals, have been criticized by Kirsten and Toms [7]. Instead, they propose to evaluate the sum directly by contour integration. In turns out, however, that this method is difficult to use in the transition region where they are forced to fall back upon a direct, numerical summation. Their results are thus quite similar to those of Grossmann and Holthaus [6].

The standard method for summing a series like (3) is Euler-Maclaurin summation [8]. One then has

\[
\sum_{n=a}^{n=b} f(n) = \int_{x=a}^{x=b} dx f(x) + \frac{1}{2} [f(b) + f(a)] + \frac{1}{12} [f'(b) - f'(a)] + \cdots
\] (5)

In our case the contributions from the upper limit will vanish. When \( T \gg h\omega/k_B \) we can also safely ignore the contributions coming from the higher order derivatives at the lower integration limit. The sum (3) can then be written as

\[
N_e = G_3(\lambda) + \frac{3}{2} G_2(\lambda) + G_1(\lambda) + \frac{1}{4} \frac{\lambda}{1 - \lambda} \left( \frac{31}{6} + \frac{b}{1 - \lambda} \right)
\] (6)

when we only include terms up to the first derivative. We have here introduced the new functions

\[
G_{p+1}(\lambda) = \frac{1}{p!} \int_1^{\infty} dx x^p \frac{\lambda e^{-bx}}{1 - \lambda e^{-bx}}
\] (7)
In the case of Bose-Einstein condensation in zero potential, the lower limit would have been \( x = 0 \) and the functions would be equal to the \( g_p(\lambda) \) functions\(^\text{[9]}\). These are equal to the more standard polylogarithmic functions

\[
Li_p(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^p}
\]  

We see that \( Li_1(z) = -\ln (1 - z) \). Furthermore we will need \( Li_p(1) = \zeta (p) \). By a partial integration one finds that the functions \((\text{7})\) can be obtained from the simple recursion relation

\[
G_{p+1}(\bar{\lambda}) = \frac{1}{b p!} Li_1(\bar{\lambda}) + \frac{1}{b} \int_{0}^{\bar{\lambda}} \frac{d\lambda}{\lambda} G_p(\lambda)
\]  

Since derivatives of polylogarithmic functions satisfy \( Li'_{p+1}(z) = Li_p(z)/z \), the new functions \((\text{7})\) can all be expressed by these. With the result \((\text{8})\) for the number of excited particles we then have

\[
N = \frac{\lambda}{1 - \lambda} + \frac{1}{b^2} Li_3(\lambda e^{-b}) + \frac{5}{2b^2} Li_2(\lambda e^{-b}) + \frac{3}{b} Li_1(\lambda e^{-b}) + b \int_{0}^{\bar{\lambda}} \frac{d\lambda}{\lambda} G_p(\lambda)
\]  

This equation determines the critical behaviour of the system.

At temperatures below the semiclassical transition temperature \((\text{4})\) most of the particles are in the condensate consisting of \( N_0 \) particles in the ground state of the harmonic oscillator. The fugacity \( \lambda \approx 1 \) follows from

\[
\lambda = \frac{N_0}{N_0 + 1}
\]  

when \( N_0 \gg 1 \). For higher temperatures we must use the full equation \((\text{10})\) to calculate \( \lambda \). The result is shown in Fig. \[\text{1}\] for \( N = 2000 \) and \( N = 20\,000 \) particles. We see that when the number of particles gets to be very large, the transition into the ground state marked by having \( \lambda = 1 \), becomes correspondingly sharp. In contrast, the effective fugacity \( \bar{\lambda} < 1 \) at all temperatures as is clearly seen from Fig. \[\text{2}\]. The number of excited particles and as we will see, also the specific heat will thus be exponentially suppressed at very low temperatures.

Above the transition temperature \((\text{4})\) the two fugacities can be taken to be equal to a very good accuracy. This corresponds to having the parameter \( b \ll 1 \) in this temperature region. The leading terms in the number of excited particles \( N_e \) are the second and third terms in \((\text{10})\), i.e.

\[
N_e = \frac{1}{b^2} Li_3(\lambda e^{-b}) + \frac{5}{2b^2} Li_2(\lambda e^{-b}) + \mathcal{O}(1/b)
\]  

\[\text{3}\]
Figure 1: The fugacity $\lambda$ as a function of $T/T_0$ for $N = 2000$ and $N = 20000$. $\lambda$ is close to unity at low temperature and starts to fall off rapidly around $T = T_0$. As $N$ is increased, the transition sharpens and the curve approaches the semiclassical result.

Expanding the polylogarithms around $b = 0$ we then get

$$N_e = \frac{1}{b^3} Li_3(\lambda) + \frac{3}{2b^2} Li_2(\lambda) + O(1/b)$$

The two first terms here are the same as obtained in the calculation of Grossmann and Holthaus[6]. They were obtained from a density of states based upon only the first two terms in the quantum mechanical degeneracy $g_n = (n^2 + 3n + 1)/2$. Their results are in surprisingly good agreement with the exact numerical results near and above the transition temperature. This is to a large extent explained by an apparent compensation of their neglect of the third term in the degeneracy by taking the integration from $n = 0$ instead of from $n = 1$. Their results thus depend on the ordinary fugacity $\lambda$ instead of the effective fugacity $\bar{\lambda}$ which appears in our more accurate analysis. As we have seen, it is the exponentially damped effective fugacity which determines the thermodynamics at very low temperatures.

In the transition region we can use the approximate result (13) for the number of ex-
Figure 2: The effective fugacity $\bar{\lambda}$ as a function of $T/T_0$ for $N = 2000$ and $N = 20000$. $\bar{\lambda}$ is always less than unity and vanishes at absolute zero. The maximum reached near the transition is seen to sharpen as $N$ is increased.

cited particles. The number of particles in the condensate thus varies with the temperature as

$$N_0 = N - \left(\frac{k_B T}{\hbar \omega}\right)^3 \zeta(3) - \frac{3}{2} \left(\frac{k_BT}{\hbar \omega}\right)^2 \zeta(2)$$ (14)

Defining the transition temperature $T_c$ where $N_0 = 0$ we see that is is given by

$$T_c = T_0 \left[ 1 - \frac{3\zeta(2)}{2N} \left(\frac{k_B T_C}{\hbar \omega}\right)^2 \right]^{1/3}$$

$$\approx T_0 \left[ 1 - \frac{\zeta(2)}{2\zeta(3)^{2/3}} \frac{1}{N^{1/3}} \right]$$

as obtained by Grossmann and Holthaus[6]. When the number of particles in the trap becomes very large, the transition temperature approaches the semiclassical result (4).
Similarly, we get for the variation of the condensate near the transition temperature,

\[ \frac{N_0}{N} = 1 - \left( \frac{T}{T_0} \right)^3 - \frac{3\zeta(2)}{2\zeta(3)^{2/3}} \frac{1}{N^{1/3}} \left( \frac{T}{T_0} \right)^2 \]  

(15)

This result is only approximately correct near the transition region where the effective fugacity \( \lambda \approx 1 \). A more accurate result is obtained by numerically solving (10) for \( \lambda \).

![Figure 3](image-url)

**Figure 3:** The condensate ratio \( \frac{N_0}{N} \) as a function of \( \frac{T}{T_0} \) for \( N = 20000 \) just below the transition. The approximate results are seen to approach the exact numerical results as more terms in Eq. (10) are included. When the third derivative in the Euler-Maclaurin formula is included, a numerical agreement to five decimal places is obtained.

The result is shown in Fig. 3 which gives the variation of the condensate just below the transition temperature. We see there the limited accuracy of just including the first two terms in \( N_e \) when comparing to the exact result obtained by numerical summation. Using the Euler-Maclaurin formula up to and including the third-derivative term, we find a numerical agreement to five decimal digits. In Fig. 4 we show the condensate varying with the temperature down to absolute zero. As \( T \to 0 \) the exponential suppression of excited particles becomes stronger and stronger. In fact, when \( T < \frac{\hbar \omega}{k} \), essentially all the excited particles will be in the \( n = 1 \) energy level of the oscillator. We then have

\[ N_0 = N - 3e^{-\frac{\hbar \omega}{k}T} \]  

(16)
when we neglect more exponentially suppressed terms.

Figure 4: The condensate ratio $N_0/N$ as a function of $T/T_0$ for $N = 2000$ and $N = 20000$. $N_0$ approaches $N$ exponentially at extremely low temperatures. Near $T = T_0$ the sharp transition found with the semiclassical approximation is rounded off by higher order corrections. In the figure one can not distinguish between the analytical and numerical results.

The specific heat is obtained from the internal energy

$$U = \sum_{n=0}^{\infty} g_n \varepsilon_n e^{\beta(\varepsilon_n - \mu)} - 1$$

In the condensate each particle has zero energy so that the sum really starts at the first excited level with $n = 1$. Again using the Euler-Maclaurin formula (5) we obtain

$$\frac{U}{\hbar \omega} = \frac{3}{b^4} Li_4(\lambda e^{-b}) + \frac{6}{b^3} Li_3(\lambda e^{-b}) + \frac{11}{2b^2} Li_2(\lambda e^{-b}) + \frac{3}{b} Li_1(\lambda e^{-b})$$

$$+ \frac{1}{41 - \lambda e^{-b}} \left( \frac{25}{6} + \frac{b}{1 - \lambda e^{-b}} \right)$$

The specific heat can now be obtained as a function of the fugacity by taking the partial derivative with respect to temperature. It will depend on the partial derivative $(\partial \lambda/\partial T)$.
which can be obtained from (10). The result is shown in Fig. 5 for different numbers of particles in the trap together with exact numerical results. At extremely low temperatures the number of excited particles is exponentially small which will thus result in a correspondingly suppressed specific heat.

\[ C_V / N k_B \]

**Figure 5:** The specific heat \( C_V / N \) as a function of \( T / T_0 \) for \( N = 2000 \) and \( N = 20000 \). The discontinuity in the specific heat found with the semiclassical approximation is smoothened by the corrections. The sharpness of the peak is seen to increase with \( N \).

When the number of trapped particles is very large, the first term in (18) gives the dominant contribution to the result. As a rough approximation, we can keep only this and setting \( \bar{\lambda} \simeq 1 \) just below the transition temperature, we have

\[
\frac{U}{\hbar \omega} \simeq 3 \left( \frac{k_B T}{\hbar \omega} \right)^4 \zeta(4) \tag{19}
\]

The specific heat at the transition temperature is thus approximately

\[
\frac{C_V}{N k_B} \simeq 12 \frac{\zeta(4)}{\zeta(3)} \tag{20}
\]

i.e. almost a factor four larger than for a classical gas in the oscillator potential.

By the same Euler-Maclaurin method we have also investigated the anisotropic oscillator trap where the frequencies \( \omega_x, \omega_y \) and \( \omega_z \) are all different [10]. Instead of the above
parameter $b$, we now introduce the three parameters $b_i = \frac{h \omega_i}{k_B T}$. Corresponding to equation (13), we then find for the first two leading terms in the result for the number of excited particles,

$$N_e = \frac{1}{b_x b_y b_z} Li_3(\lambda) + \frac{1}{2} \left( \frac{1}{b_x b_y} + \frac{1}{b_y b_z} + \frac{1}{b_x b_z} \right) Li_2(\lambda) + \ldots$$  \hspace{1cm} (21)

Grossmann and Holthaus[6] considered a potential with $\omega_x = 600$ Hz, $\omega_y = \sqrt{2} \omega_x$ and $\omega_z = \sqrt{3} \omega_x$. They write the coefficient of $Li_2(\lambda)$ as $\gamma (k_B T / \hbar \omega)^2$ where $\omega = (\omega_x \omega_y \omega_z)^{1/3}$ and find $\gamma \approx 1.6$ from a numerical summation over the energy levels of the anisotropic oscillator. On the other hand, we obtain from (21)

$$\gamma = \left( \frac{3}{4} \right)^{1/3} \left( \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{6}} \right) \approx 1.538$$  \hspace{1cm} (22)

which agrees quite well with their approximate result.

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