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Finite-size effects on the Bose–Einstein condensation critical temperature in a harmonic trap

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ABSTRACT

We obtain second and higher order corrections to the shift of the Bose–Einstein critical temperature due to finite-size effects. The confinement is that of a harmonic trap with general anisotropy. Numerical work shows the high accuracy of our expressions. We draw attention to a subtlety involved in the consideration of experimental values of the critical temperature in connection with analytical expressions for the finite-size corrections.

1. Introduction

In the first realizations of Bose–Einstein condensation (BEC) in the laboratory [1–3] and in many experiments ever since, the Bose gas is trapped in a potential that can be considered as parabolic to a very good approximation. In the thermodynamic limit, within the ideal gas approximation, the critical temperature for such a system is given by $k_B T_0 = (N/\zeta(3))^{1/3}\hbar\tilde{\omega}$, where $\tilde{\omega} = (\omega_x\omega_y\omega_z)^{1/3}$ is the geometric mean of the trap frequencies and all the other symbols have their usual meaning (see e.g. [4]). Soon after the first experiments, corrections to this expression, $\Delta T_c \equiv T_c - T_0$, were found. On the one hand, experiments do not take place in the thermodynamic limit. Hence, finite-size corrections are required. On the other hand, the gases are not ideal, having a non-vanishing scattering length. Hence, interaction effects must be taken into account.

The first order shift ΔT_c due to interactions was determined analytically early on in [5] within a mean-field approximation, in the form of a linear term in the scattering length. Higher order corrections followed in several works [6–16], both numerical and analytical. Expansions for ΔT_c in powers of the scattering length down to second order were determined, both within a mean-field approach [9,17,12,15,16] and accounting for critical correlations [7].

The first order finite-size induced shift was given in the isotropic case in [18,19] and in the general anisotropic case in [20] as

$$\Delta T_c = -\frac{\zeta(2)}{2\zeta(3)}\frac{\hbar\bar{\omega}}{k_B}, \tag{1}$$

where $\bar{\omega} = (\omega_x + \omega_y + \omega_z)/3$. More recently, a higher order result was given in [21] (see also [22,23]). This result relies on the local density approximation, in which the discrete energy levels of the finite system are approximated by a continuum, therefore requiring that the typical thermal energy at the transition be much greater than the typical inter-level spacing (for example, in the case of an isotropic harmonic trap, $k_B T_c \gg \hbar\omega$), i.e., the thermodynamic limit. Moreover, in order to overcome the vagueness (or non-point-like character) associated with the critical temperature of the finite system, we believe it would be useful to consider an explicit physical criterion for this critical temperature, related for example to the condensate fraction or the specific heat, when going to the level of detail of higher-order corrections [22].

Strictly speaking, a finite-size correction to T_0 is an ill-defined concept when taken on its own because the effect of finite size is to spread out the phase transition from a point to a narrow temperature interval. The first order correction (1) is typically extracted from a high temperature finite-size expansion of the number of particles, which takes into due account the discreteness of the energy levels and which can be obtained in several ways [20, 24–26]. If one attempts to find a second order correction from this expansion, the absence of a true critical temperature makes itself noticed: the next order term in the expansion is divergent at the critical point, ultimately implying the non-existence of BEC as a sharp, mathematically defined phase transition in finite systems. It follows that the first order corrected T_c must not be taken too seriously. It merely provides a reference value for signaling the transition.

In experimental work where the BEC critical temperature is measured [27–30], the expression generally quoted for purposes of comparison with theory, namely for splitting off finite-size ef-

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fects from interaction effects, is the one in (1). Now, as mentioned above, this expression should not be taken at face value. Thus, there is the possibility that a misinterpretation of the finite-size related shift can lead to a bias in the reported values of the interaction induced shift. It would be of interest to make this matter clearer. What is actually measured in experiments is the number of particles, ground state fraction, trap frequencies and temperature. It is by performing some polynomial fit to a plot involving these quantities that an experimental value for T_c is usually extracted [27–29]. In the landmark experiment reported in [28] the fit is performed in the region where the condensate fraction "noticeably starts to increase". Condensate fractions as low as about 1% could be measured in this experiment. If lower condensate fractions could be measured, higher critical temperatures would have been obtained, even rising above T_0 for sufficiently small condensate fractions. This is because for finite systems the condensate fraction is not zero for temperatures above the critical region. It is just very small. This fact becomes more conspicuous for low particle numbers. Another major experiment in what concerns high precision measurements of T_c is reported in [29]. Here, very much the same comments apply. In this case, condensate fractions as low as 0.1% could be detected. The authors overcome the problem of isolating interaction from finite-size corrections by performing differential measurements with reference to a standard value of the scattering length. Nevertheless, as recently pointed out [12], this assumes that finite size and interaction effects are independent. At second order, it might not be the case.

Our aim in the present work is to obtain higher-order finite-size corrections to the critical temperature of a Bose gas in a general harmonic trap. To do this in a meaningful way, which at the same time can connect to experimental procedures, we overcome the non-existence of a true critical temperature by asking instead for the temperature T_κ at which the condensate fraction has a given small value $N_{\rm gr}/N = \kappa$, $\kappa \ll 1$. Other criteria could be used, like defining T_c by the maximum of the specific heat or the inflection point of the $N_{\rm gr}(T)$ curve; but the one we adopt here is probably the most useful because it uses the condensate fraction and it is very simple. From the well known bulk behaviour of the condensate fraction in the BEC regime, $N_{\rm gr}/N = 1-(T/T_0)^3$, we have in the thermodynamic limit $T_\kappa/T_0 = (1-\kappa)^{1/3}$. For $\kappa \to 0$, this yields $T_\kappa \to T_0$. We will provide finite-size corrections to T_κ down to third order. Stopping at second order is not accurate enough in some circumstances, as detailed below. Our approach preserves all the finite-size characteristics of the system, with no approximations involved. The information on the discrete structure of the energy levels is carried in the expansions (4) and (5) below. Finally, we note that our expressions are also valid (and highly accurate) for κ not small, i.e., deep into the BEC regime.

2. Finite-size corrections

Let $x = \beta\hbar\bar{\omega} = \hbar\bar{\omega}/(k_B T)$ and $\epsilon = (E_{\rm gr}-\mu)/(\hbar\bar{\omega})$. x is a rescaled inverse temperature and ϵ can be looked at as a rescaled chemical potential. We define the anisotropy vector $\boldsymbol{\lambda} = (\lambda_1,\lambda_2,\lambda_3) = (\omega_1,\omega_2,\omega_3)/\bar{\omega}$. Using grand-canonical statistics, the number of particles N of an ideal Bose gas in this trap is given by

$$N = \sum_{\mathbf{n}} \left[e^{\beta(E_{\mathbf{n}}-\mu)} - 1 \right]^{-1} = \sum_{\mathbf{n}} \sum_{k=1}^{\infty} e^{-kx(\boldsymbol{\lambda}\cdot\mathbf{n}+\epsilon)} . \tag{2}$$

The sum in $\mathbf{n}$ is over all single particle states, of energy $E_{\mathbf{n}} = \sum_{i=1}^{3}(n_i+1/2)\hbar\omega_i$, $n_i = 0,1,2,\ldots$. Let $\lambda = (\lambda_1\lambda_2\lambda_3)^{1/3}$. The usual bulk result for N, which is exact in the thermodynamic limit, reads in our variable $x^3 N = {\rm Li}_3(e^{-x\epsilon})\lambda^{-3}$ if $T \geq T_0$ and $x^3 N = x^3 N_{\rm gr} + \zeta(3)\lambda^{-3}$ if $T < T_0$ (where $x^3 N$ is the quantity that remains finite in the thermodynamic limit, as opposed to N). ${\rm Li}_3$ is the polylogarithm of index 3, with the property ${\rm Li}_3(1) = \zeta(3)$. Define $x_0 = \hbar\bar{\omega}/(k_B T_0) = (\zeta(3)/N)^{1/3}\lambda^{-1}$. As we approach the thermodynamic limit in the usual way ($N\omega_i^3$ kept fixed) we have $x_0 \to 0$, or for any fixed temperature, $x \to 0$. x and eventually x_0 will be our expansion parameters. In the BEC regime, we have in addition (still in the thermodynamic limit) $N_{\rm gr} = 1/(\epsilon x)$, from where we see that ϵ scales as x^2.

What we need is an expansion for N that contains the finite-size corrections and that is valid *throughout* the critical region. This can be achieved by applying a Mellin–Barnes transform to the exponential inside the k summation in (2), as indeed was done before in [31]. The same procedure was also applied to a Bose gas subject to other confinements [32,33]. An expansion is obtained by solving a contour integral in the complex plane using the theorem of residues. In this case, the Riemann and three-dimensional Barnes zeta functions, here denoted $\zeta(\alpha)$ and $\zeta_B(\alpha,\epsilon|\boldsymbol{\lambda})$ respectively, make their appearance. Knowledge of the residues at the poles of these functions is required. We refer the reader to [31] for details of the procedure. ζ_B is a multi-dimensional generalization of the Hurwitz zeta function, which was studied in depth by Barnes in [34] (see also [35]). In [31] the expansion for N was calculated to subleading order. However, for our purposes we need also the third and fourth terms. The calculation of the third term, in particular, is more involved due to the existence of a double pole, requiring the knowledge of the finite part at the $\alpha = 1$ pole of $\zeta_B(\alpha,\epsilon|\boldsymbol{\lambda})$, not only its residue. Specifically, below we need the quantity $b_0(\boldsymbol{\lambda})$ defined in the following way. Let $a_0(\epsilon|\boldsymbol{\lambda})$ be the finite part at the $\alpha = 1$ pole of $\zeta_B(\alpha,\epsilon|\boldsymbol{\lambda})$. Then $b_0 = \lim_{\epsilon\to 0}(a_0(\epsilon|\boldsymbol{\lambda}) - \epsilon^{-1})$, i.e., $a_0(\epsilon|\boldsymbol{\lambda}) = \epsilon^{-1} + b_0 + \mathcal{O}(\epsilon)$. b_0 is a function of $\boldsymbol{\lambda}$ only. We obtain the expansion

$$\begin{aligned} N = {} & \frac{\zeta(3)}{\lambda^3}x^{-3} + \frac{3-2\epsilon}{2\lambda^3}\zeta(2)x^{-2} \\ & + \left[a_0(\epsilon|\boldsymbol{\lambda}) - \frac{9+(\lambda_i\lambda_j)-18\epsilon+6\epsilon^2}{12\lambda^3}\ln x \right] x^{-1} \\ & - \frac{1}{2}\zeta_B(0,\epsilon|\boldsymbol{\lambda}) + \mathcal{O}(x) , \end{aligned} \tag{3}$$

where we have adopted the following notational conventions: $(\lambda_i\lambda_j) = \sum_{i,j=1\,(i<j)}^{3}\lambda_i\lambda_j = \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3$ and $(\lambda_i^2\lambda_j) = \sum_{i,j=1\,(i\neq j)}^{3}\lambda_i^2\lambda_j$. The first two terms in (3) were given in [31]. From [34] we have that $\zeta_B(0,\epsilon|\boldsymbol{\lambda}) = 1/8 + (\lambda_i^2\lambda_j)/(24\lambda^3) + \mathcal{O}(\epsilon)$. The full asymptotic expansion for N could easily be given, but it is not needed.

Define the rescaled temperature $t = T/T_0 = x_0/x$. In (3), change from the variables N, x and ϵ to x_0, t and ϵ by performing the substitutions $N = \zeta(3)/(\lambda x_0)^3$ and $x = x_0/t$. Equation (3) gives us ϵ implicitly as a function of x_0 and t. Since $\epsilon = \mathcal{O}(x_0^2)$ for $t < 1$, we solve for ϵ perturbatively by letting $\epsilon = a(t)x_0^2 + b(t)x_0^3 + c'(t)x_0^4\ln x_0 + c(t)x_0^4 + \cdots$ and find the coefficients $a(t), b(t)\ldots$. Next we use the expression for the condensate fraction $N_{\rm gr}/N = (e^{\epsilon x}-1)^{-1}/N$. In this expression, we change again to the variables x_0, t and ϵ and substitute the newly found expansion for ϵ. Expanding the resulting expression in powers of x_0 yields

$$\begin{aligned} \frac{N_{\rm gr}}{N} = {} & \left(1-t^3\right) - \frac{3\zeta(2)}{2\zeta(3)}t^2 x_0 \\ & - \frac{\lambda^3 t}{\zeta(3)}\left[b_0 + \frac{9+(\lambda_i\lambda_j)}{12\lambda^3}(\ln t - \ln x_0) \right] x_0^2 \\ & + \frac{\lambda^3}{\zeta(3)}\left[\frac{\zeta(2)}{\zeta(3)}\frac{t^3}{1-t^3} + \frac{(\lambda_i^2\lambda_j)}{48\lambda^3} - \frac{7}{16} \right] x_0^3 + \cdots . \end{aligned} \tag{4}$$

This equation gives us the condensate fraction as a function of t and N (or t and x_0). It is valid throughout the BEC regime and