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B. Klünder and A. Pelster



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B. Klünder¹ and A. Pelster^{2,a}

¹ Arnold Sommerfeld Center for Theoretical Physics, Fakultät für Physik, Ludwig-Maximilians-Universität München, Theresienstrasse 37, 80333 München, Germany

² Universität Duisburg-Essen, Fachbereich Physik, Campus Duisburg, Lotharstrasse 1, 47057 Duisburg, Germany

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Abstract. Using a field-theoretic approach, we systematically generalize the usual semiclassical approximation for a harmonically trapped ideal Bose gas in such a way that its range of applicability is essentially extended. With this we can analytically calculate thermodynamic properties even for small particle numbers. In particular, it now becomes possible to determine the critical temperature as well as the temperature dependence of both heat capacity and condensate fraction in low-dimensional traps, where the standard semiclassical approximation is not even applicable.

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1 Introduction

The field of ultracold Bose gases attains at present a lot of attention due to an improved experimental accessibility within the last decade. Many different theoretical approaches are used to treat these trapped dilute quantum gases. Although isolated Bose gases should, in principle, be described within the micro-canonical ensemble, one commonly applies the technically more efficient canonical or grand-canonical descriptions [1–20]. This is justified as experiments often use a large number of bosons. It is a common belief in quantum statistics that, at least in the thermodynamic limit $N \rightarrow \infty$, all ensembles should converge to one and the same result. However, we note that some peculiar exceptions are known for particle counting statistics as discussed, for instance, in references [20–22]. From a theoretical point of view, the grand-canonical ensemble has the advantage that it provides an analytical description, whereas the canonical approach is limited to numerical results for moderate particle numbers. As experiments with ultracold Bose gases are always realised with a finite number of particles, the fundamental question arises how to study finite-size effects for the thermodynamic properties of trapped Bose gases most efficiently.

To analyse this problem systematically, we introduce and compare two different approaches. In Section 2 we briefly rederive the well-known grand-canonical

description without using the order parameter concept for a harmonically confined ideal Bose gas. The thermodynamic properties can only be calculated numerically in this theory. In Section 3 we introduce another grand-canonical description of the trapped Bose gas which is analytical as it relies on the order parameter concept. Introducing an order parameter is an essential approximation for finite systems and leads to different results for the respective thermodynamic quantities compared to the theory without order parameter. However these differences vanish in the thermodynamic limit and turn out to be negligibly small for experimentally realistic system sizes. Moreover, generalizing a formalism developed in reference [23], Appendix 7A, this approach extends the usual semiclassical approximation [1,2,13,16] to a systematic semiclassical expansion which yields yet unknown analytical results for the thermodynamic quantities in the superfluid phase. In particular, we will calculate the critical temperature T_c as well as the temperature dependence of the condensate fraction N_0/N and the heat capacity C_V for $D = 1, 2, 3$ dimensions up to the order of the semiclassical expansion which was not accessible before.

2 Approach without order parameter

We start with briefly rederiving the well-known grand-canonical description of an ideal Bose gas. The general

^a e-mail: axel.pelster@uni-due.de

expression for the grand-canonical potential of an ideal Bose gas is given by [24]

$$\Omega = \frac{1}{\beta} \sum_{\mathbf{n}} \log \left[1 - e^{-\beta(E_{\mathbf{n}} - \mu)} \right], \quad (1)$$

where \mathbf{n} describes the one-particle quantum numbers. Here $E_{\mathbf{n}}$, $\beta = 1/k_B T$, and μ denote the energy levels of the system, the inverse temperature, and the chemical potential, respectively. We specify equation (1) for the case of an ideal Bose gas which is trapped in an isotropic harmonic potential of the form $V(\mathbf{x}) = M\omega^2 \mathbf{x}^2/2$, where M and ω denote the mass of a bosonic particle and the trap frequency, respectively. The one-particle energy eigenvalues of a harmonic oscillator are $E_{\mathbf{n}} = \hbar\omega(n_1 + \dots + n_D + D/2)$ in D dimensions, so the grand-canonical potential (1) specifies to

$$\Omega = -\frac{1}{\beta} \sum_{k=1}^{\infty} \frac{e^{\beta(\mu - E_0)k}}{k(1 - e^{-\hbar\omega\beta k})^D}. \quad (2)$$

For numerical calculations it turns out to be useful to follow reference [25] and reexpress (2) by using the polylogarithms

$$\zeta_a(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^a} \quad (3)$$

and the identity

$$\frac{1}{(1-z)^D} = \sum_{m=0}^{\infty} \binom{m+D-1}{m} z^m, \quad (4)$$

so we obtain

$$\Omega = -\frac{1}{\beta} \sum_{m=0}^{\infty} \binom{m+D-1}{m} \zeta_1 \left(e^{\beta(\mu - E_0 - m\hbar\omega)} \right). \quad (5)$$

With $N = -\partial\Omega/\partial\mu$ one gets for the particle number equation

$$N = \sum_{m=0}^{\infty} \binom{m+D-1}{m} \zeta_0 \left(e^{\beta(\mu - E_0 - m\hbar\omega)} \right), \quad (6)$$

which can be solved numerically for the chemical potential μ once the particle number N is given. In this approach we consider the resulting condensate fraction

$$\frac{N_0}{N} = \frac{1}{N[e^{\beta(E_0 - \mu)} - 1]} \quad (7)$$

as a function of the temperature and define the point where the curvature is maximal as the critical temperature T_c . Figure 1 shows the chemical potential μ in $D = 3$ dimensions determined from (6) as a function of temperature T for a given particle number N . One observes that μ remains smaller than the ground-state energy E_0 for all temperatures and approaches E_0 in the limit $T \downarrow 0$. Moreover, one can see that $(\mu - E_0)/\hbar\omega$ gets smaller for $T \leq T_c$ if the particle number N is increased.

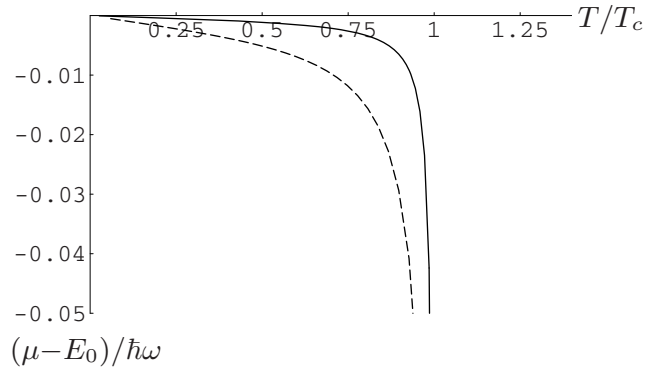


Fig. 1. Dimensionless chemical potential $(\mu - E_0)/\hbar\omega$ versus T/T_c in $D = 3$ dimensions determined from (6) for $N = 10^3$ particles (dashed line) and $N = 10^4$ (solid line) for $\omega = 2\pi \cdot 40$ Hz. The critical temperatures are $T_c = 16.75$ nK for $N = 10^3$ and $T_c = 37.56$ nK for $N = 10^4$, respectively.

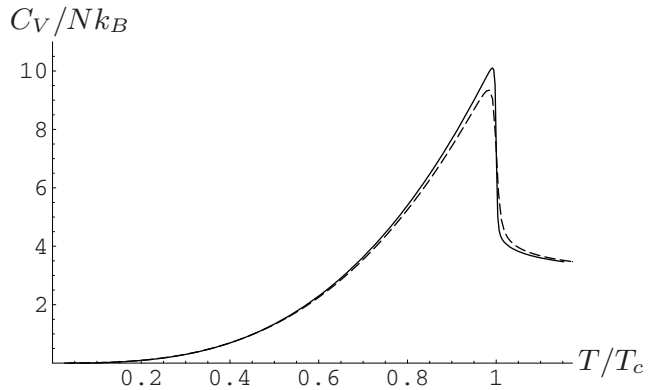


Fig. 2. Heat capacity (8) versus T/T_c in $D = 3$ dimensions for $N = 10^4$ (dashed line) and $N = 10^5$ (solid line) for $\omega = 2\pi \cdot 40$ Hz. The critical temperatures are $T_c = 37.56$ nK for $N = 10^4$ and $T_c = 82.46$ nK for $N = 10^5$, respectively.

The heat capacity $C_V = \partial U/\partial T|_{V,N}$ is derived from the internal energy $U = \Omega + TS + \mu N$ and yields

$$C_V = k_B(\hbar\omega\beta)^2 \times \sum_{m=0}^{\infty} m \binom{m+D-1}{m} \zeta_{-1} \left(e^{\beta(\mu - E_0 - m\hbar\omega)} \right) \times \left[m - \frac{\sum_{m'=0}^{\infty} m' \binom{m'+D-1}{m'} \zeta_{-1} \left(e^{\beta(\mu - E_0 - m'\hbar\omega)} \right)}{\sum_{m''=0}^{\infty} \binom{m''+D-1}{m''} \zeta_{-1} \left(e^{\beta(\mu - E_0 - m''\hbar\omega)} \right)} \right]. \quad (8)$$

One can see in Figure 2 that C_V in $D = 3$ dimensions has its maximum at $T \approx T_c$ and vanishes exponentially fast in the limit $T \downarrow 0$. The heat capacity C_V gets larger for $T \leq T_c$ and smaller for $T > T_c$ if the particle number N is increased. Moreover, one obtains that the slope at $T = T_c$ increases as well for larger N , but does not diverge. With this we have shown exemplarily that phase transitions do not occur in finite systems. However, μ and C_V for fixed T/T_c seem to tend towards a limit for large

particle numbers N and thus, we expect the emergence of a sharp phase transition in the thermodynamic limit $N \rightarrow \infty$. In the next section we use this observation as a motivation to introduce an analytical approach for describing a trapped Bose gas with the help of an order parameter.

3 Approach with order parameter

We start with the functional integral approach to the grand-canonical partition function of a harmonically trapped ideal Bose gas [26]

$$Z = \oint \mathcal{D}\psi^* \mathcal{D}\psi e^{-\mathcal{A}[\psi^*, \psi]/\hbar}, \quad (9)$$

where one integrates over all possible bosonic Schrödinger fields $\psi^*(\mathbf{x}, \tau), \psi(\mathbf{x}, \tau)$ which are periodic in imaginary time τ with period $\hbar\beta$. The Euclidean action $\mathcal{A}[\psi^*, \psi]$ reads

$$\begin{aligned} \mathcal{A}[\psi^*, \psi] &= \int_0^{\hbar\beta} d\tau \int d^D x \psi^*(\mathbf{x}, \tau) \\ &\times \left[\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \Delta}{2M} + \frac{M}{2} \omega^2 \mathbf{x}^2 - \mu \right] \psi(\mathbf{x}, \tau). \end{aligned} \quad (10)$$

We evaluate the functional integral by using the background method [27,28]. To this end we divide the fields $\psi^*(\mathbf{x}, \tau), \psi(\mathbf{x}, \tau)$ into field expectation values $\Psi^*(\mathbf{x}, \tau), \Psi(\mathbf{x}, \tau)$, which we identify later on with the macroscopic occupation of the ground state, and fluctuations $\delta\psi^*(\mathbf{x}, \tau), \delta\psi(\mathbf{x}, \tau)$:

$$\begin{aligned} \psi^*(\mathbf{x}, \tau) &= \Psi^*(\mathbf{x}, \tau) + \delta\psi^*(\mathbf{x}, \tau), \\ \psi(\mathbf{x}, \tau) &= \Psi(\mathbf{x}, \tau) + \delta\psi(\mathbf{x}, \tau). \end{aligned} \quad (11)$$

Note that field expectation values and fluctuations have to satisfy the condition [29]

$$\int d^D x \Psi^*(\mathbf{x}, \tau) \delta\psi(\mathbf{x}, \tau) = 0. \quad (12)$$

Using (11) together with (9) we arrive at

$$Z = e^{-\mathcal{A}[\Psi^*, \Psi]/\hbar} \oint \mathcal{D}\delta\psi^* \mathcal{D}\delta\psi e^{-\mathcal{A}[\delta\psi^*, \delta\psi]/\hbar}. \quad (13)$$

Now we decompose the fluctuations $\delta\psi(\mathbf{x}, \tau)$ into the one-particle eigenstates $\psi_{\mathbf{n}}(\mathbf{x})$ of the system and apply an additional Matsubara decomposition:

$$\delta\psi(\mathbf{x}, \tau) = \sum_{\mathbf{n} \neq 0} \sum_{m=-\infty}^{\infty} c_{\mathbf{n}, m} \psi_{\mathbf{n}}(\mathbf{x}) \frac{e^{-i\omega_m \tau}}{\sqrt{\hbar\beta}} \quad (14)$$

with the Matsubara frequencies $\omega_m = 2\pi m/\hbar\beta$. Note that we explicitly do not sum over the ground state of the system in (14), as we have to satisfy condition (12). With

this, the measure of the functional integration (13) turns into

$$\oint \mathcal{D}\delta\psi^* \mathcal{D}\delta\psi = \prod_{\mathbf{n} \neq 0} \prod_{m=-\infty}^{\infty} \int \frac{dc_{\mathbf{n}, m}^* dc_{\mathbf{n}, m}}{2\pi\hbar\beta}. \quad (15)$$

The integration over the expansion coefficients $c_{\mathbf{n}, m}^*, c_{\mathbf{n}, m}$ in (15) is now Gaussian and can be performed. The effective action is then found by applying the logarithm to the partition function: $\Gamma[\Psi^*, \Psi] = -(\log Z)/\beta$. With this one gets

$$\begin{aligned} \Gamma[\Psi^*, \Psi] &= \frac{1}{\hbar\beta} \mathcal{A}[\Psi^*, \Psi] \\ &- \frac{1}{\beta} \sum_{k=1}^{\infty} \frac{e^{\beta(\mu - E_0)k}}{k} \left[\frac{1}{(1 - e^{-\hbar\omega\beta k})^D} - 1 \right]. \end{aligned} \quad (16)$$

This effective action yields the grand-canonical potential Ω if it is evaluated for extremised field expectation values: $\Omega = \Gamma[\Psi_e^*, \Psi_e]$. An extremization of (16) with respect to $\Psi^*(\mathbf{x}, \tau)$ leads to

$$\left\{ \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \Delta}{2M} + \frac{M}{2} \omega^2 \mathbf{x}^2 - \mu \right\} \Psi_e(\mathbf{x}, \tau) = 0. \quad (17)$$

This equation has the eigenstates $\psi_{\mathbf{n}}(\mathbf{x})$ with $\mu = E_{\mathbf{n}}$ as non-trivial solutions which are periodic in imaginary time. We choose the ground state $\psi_0(\mathbf{x}) = (M\omega/\pi\hbar)^{D/4} \exp(-M\omega\mathbf{x}^2/2\hbar)$ to be the physically meaningful solution and normalise $\Psi_e(\mathbf{x}, \tau)$ to the number of atoms in the ground state N_0 :

$$\Psi_e(\mathbf{x}, \tau) = \sqrt{N_0} \psi_0(\mathbf{x}). \quad (18)$$

As (17) and (18) lead to the algebraic equation

$$(E_0 - \mu) \sqrt{N_0} = 0, \quad (19)$$

we obtain two different phases. In the gas phase we have $N_0 = 0$, whereas in the superfluid phase with $N_0 \neq 0$ the chemical potential μ must be equal to the ground-state energy E_0 . The critical temperature T_c occurs at the borderline between both phases, so it follows from the particle number equation by setting both $N_0 = 0$ and $\mu = E_0$. To this end we combine (16) and (18) and get for the grand-canonical potential

$$\begin{aligned} \Omega &= (E_0 - \mu) N_0 \\ &- \frac{1}{\beta} \sum_{k=1}^{\infty} \frac{e^{\beta(\mu - E_0)k}}{k} \left[\frac{1}{(1 - e^{-\hbar\omega\beta k})^D} - 1 \right]. \end{aligned} \quad (20)$$

The first term represents the contribution of the macroscopically occupied ground state of the system, whereas the second term describes the thermal contributions of all excited states. This should be compared with (2) where the ground state is treated like all other states.

4 Thermodynamics

It is now possible to derive all thermodynamic quantities from (20) within this framework. The particle number equation $N = -\partial\Omega/\partial\mu$ reads

$$N = N_0 + \sum_{k=1}^{\infty} e^{\beta(\mu-E_0)k} \left[\frac{1}{(1 - e^{-\hbar\omega\beta k})^D} - 1 \right]. \quad (21)$$

The internal energy follows from the Legendre transformation $U = \Omega + TS + \mu N$:

$$U = E_0 N_0 + D\hbar\omega \sum_{k=1}^{\infty} e^{\beta(\mu-E_0)k} \left\{ \frac{1}{2} \left[\frac{1}{(1 - e^{-\hbar\omega\beta k})^D} - 1 \right] + \frac{e^{-\hbar\omega\beta k}}{(1 - e^{-\hbar\omega\beta k})^{D+1}} \right\}. \quad (22)$$

Both the particle number N and the internal energy U can be expressed by the auxiliary functions

$$I(A, b, D) = \sum_{k=1}^{\infty} \frac{e^{-bAk}}{(1 - e^{-bk})^D}. \quad (23)$$

The particle number (21) turns into

$$N = N_0 + \sum_{l=1}^D (-1)^{l+1} \binom{D}{l} I(l - \mu', b, D), \quad (24)$$

where we have used the abbreviations $b = \hbar\omega\beta$ and $\mu' = (\mu - E_0)/\hbar\omega$. For the internal energy (22) we get correspondingly

$$U = E_0 N_0 + D\hbar\omega \left[\frac{1}{2} \sum_{l=1}^D (-1)^{l+1} \binom{D}{l} I(l - \mu', b, D) + I(1 - \mu', b, D+1) \right]. \quad (25)$$

With this it is possible to calculate useful analytic approximations for the critical temperature T_c , as well as the temperature dependence of both the condensate fraction N_0/N and the heat capacity C_V for different numbers of spatial dimensions D . To this end we assume that the difference $\hbar\omega$ between different energy levels of the harmonic oscillator is small compared to the average thermal energy $k_B T$. This yields the semiclassical condition $0 < b = \hbar\omega\beta \ll 1$, which is well fulfilled for present-day experiments.

In order to describe the superfluid phase we apply the limit $\mu \uparrow E_0$ to the particle number equation (24) for $D = 1, 2, 3$ and use the formulas (A.13)–(A.15) which are derived in the Appendix within the semiclassical approximation. Furthermore, we expand the polylogarithms for small $b = \hbar\omega\beta$ by using the Robinson formula [30]

$$\zeta_l(e^{-a}) = \frac{(-a)^{l-1}}{(l-1)!} \left\{ \sum_{k=1}^{l-1} \frac{1}{k} - \ln a \right\} + \sum_{\substack{k=0 \\ k \neq l-1}}^{\infty} \frac{(-a)^k}{k!} \zeta(l-k). \quad (26)$$

Thus, we get for $T \leq T_c$

$$N|_{D=1} = N_0 + \frac{\gamma - \ln(\hbar\omega\beta)}{\hbar\omega\beta} + \dots, \quad (27)$$

$$N|_{D=2} = N_0 + \frac{\zeta(2)}{(\hbar\omega\beta)^2} + \frac{-\ln(\hbar\omega\beta) + \gamma - 1/2}{\hbar\omega\beta} + \dots, \quad (28)$$

$$N|_{D=3} = N_0 + \frac{\zeta(3)}{(\hbar\omega\beta)^3} + \frac{3\zeta(2)}{2(\hbar\omega\beta)^2} + \frac{-\ln(\hbar\omega\beta) + \gamma - 19/24}{\hbar\omega\beta} + \dots \quad (29)$$

Here $\zeta(z)$ denotes the Riemann zeta function and $\gamma = 0.5772\dots$ is Euler's constant. Surprisingly, our results (27)–(29) coincide with the findings of two different approaches which are reviewed and compared in reference [12]. The first one is a master equation approach to canonical condensate statistics which is based on an analogy to the laser phase transition [10,19]. It yields accurate results even for small systems, is valid for all temperature, but is partly numerical. The second one, which is entirely based on considering the particle-number distribution, is fully analytical, but is limited to temperatures below T_c [11,15].

4.1 Critical temperature

Setting $N_0 = 0$ in (27)–(29), one obtains for the critical temperature

$$T_c|_{D=1} = \frac{\hbar\omega}{k_B} \frac{N}{\gamma - \ln(\hbar\omega/k_B T_c)} + \dots, \quad (30)$$

$$T_c|_{D=2} = \frac{\hbar\omega}{k_B} \left(\frac{N}{\zeta(2)} \right)^{\frac{1}{2}} \left\{ 1 - \left(\frac{\zeta(2)}{N} \right)^{\frac{1}{2}} \frac{1}{2\zeta(2)} \times \left[-\frac{1}{2} \ln \left(\frac{\zeta(2)}{N} \right) + \gamma - \frac{1}{2} \right] \right\} + \dots, \quad (31)$$

$$T_c|_{D=3} = \frac{\hbar\omega}{k_B} \left(\frac{N}{\zeta(3)} \right)^{\frac{1}{3}} \left\{ 1 - \left(\frac{\zeta(3)}{N} \right)^{\frac{1}{3}} \frac{\zeta(2)}{2\zeta(3)} - \left(\frac{\zeta(3)}{N} \right)^{\frac{2}{3}} \frac{1}{3\zeta(3)} \left[-\frac{1}{3} \ln \left(\frac{\zeta(3)}{N} \right) + \gamma - \frac{19}{24} - \frac{3\zeta(2)^2}{4\zeta(3)} \right] \right\} + \dots \quad (32)$$

In $D = 1$ dimension the critical temperature T_c follows from numerically solving the implicit equation (30). Higher corrections to (30) are of the order $\mathcal{O}(N^{-1})$, so they are small and can be neglected. Note that our result (30) differs slightly from the corresponding finding of references [2,18]. For $D = 2, 3$ one defines the thermodynamic limit $N \rightarrow \infty$ in such a way that the leading order of (31) and (32), i.e. $T_c^{(0)} = \hbar\omega N^{1/D}/k_B \zeta(3)^{1/D}$, remains constant. Thus, when the particle number N is

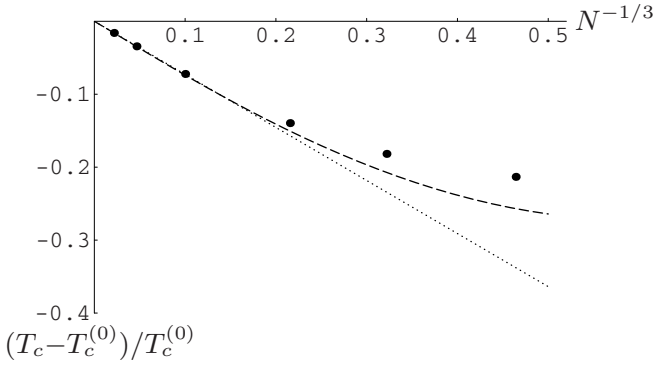


Fig. 3. Finite-size corrections $(T_c - T_c^{(0)})/T_c^{(0)}$ taken from equation (32) versus $N^{-1/3}$ for $D = 3$ dimensions. The dotted (dashed) line includes the first (the first two) finite-size correction(s). The bullets correspond to the critical temperature which is numerically determined from (6) and (7) of the theory without order parameter.

sent to infinity the trap frequency ω has to approach zero in such a way that the product $N\omega^D$ is kept fixed. In this case the quantity $b_c^{(0)} = \hbar\omega\beta_c^{(0)}$ is, indeed, small as has been assumed above. Higher orders of (31) and (32) are called finite-size corrections. We note that additional non-trivial logarithmic dependences on the particle number N occur which do not follow from the standard semiclassical approximation [1,2,13,16]. In Figure 3 the critical temperature in $D = 3$ dimensions is plotted up to the first and the second order for different particle numbers N and compared with the corresponding finite-size corrections which are obtained numerically from the theory without order parameter from (6) and (7). Combining the first and second finite-size corrections from (32) yields a better agreement with the theory without order parameter than the first finite-size correction alone. Furthermore, we read off from Figure 3 that, for particle numbers larger than about $N = 10^3$, the analytic formula (32) yields values for the critical temperature which coincide with the corresponding results of the theory without order parameter for all practical purposes. Thus, although introducing an order parameter for studying finite-size effects represents an essential approximation, its findings do not differ from the results of the theory without an order parameter for experimentally realistic system sizes. Note that the first correction of (32) was already found some time ago [1,2], whereas the second correction has only recently been found ([23], Appendix 7A).

4.2 Condensate fraction

The new feature of our approach is that it is applicable in the whole temperature regime. For instance, one gets for the condensate fraction N_0/N from (27)–(32)

$$\frac{N_0}{N}\Big|_{D=1} = 1 - \frac{T}{T_c} \left[1 - \frac{\ln(T_c/T)}{\gamma - \ln(\hbar\omega\beta_c)} \right] + \dots, \quad (33)$$

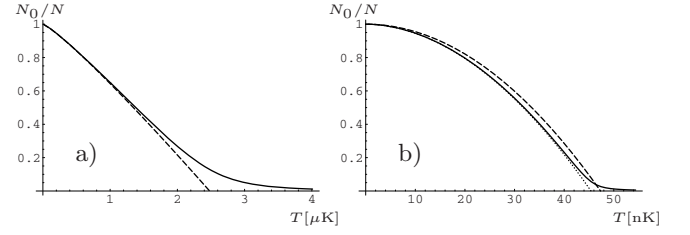


Fig. 4. Condensate fraction N_0/N versus temperature T for (a) $D = 1$ dimension and $N = 10^4$ and for (b) $D = 2$ dimensions and $N = 10^3$ for $\omega = 2\pi \cdot 40$ Hz. The solid lines describe equation (7) from the theory without order parameter, the dashed lines correspond to the leading orders of (33), (34) and the dotted line also includes the first finite-size correction.

$$\begin{aligned} \frac{N_0}{N}\Big|_{D=2} = & 1 - \left(\frac{T}{T_c}\right)^2 - \left(\frac{\zeta(2)}{N}\right)^{\frac{1}{2}} \left\{ \left[\frac{T}{T_c} - \left(\frac{T}{T_c}\right)^2\right] \right. \\ & \times \frac{-\ln(\zeta(2)/N)/2 + \gamma - 1/2}{\zeta(2)} \\ & \left. + \frac{T}{T_c} \frac{\ln(T/T_c)}{\zeta(2)} \right\} + \dots, \end{aligned} \quad (34)$$

$$\begin{aligned} \frac{N_0}{N}\Big|_{D=3} = & 1 - \left(\frac{T}{T_c}\right)^3 - \left(\frac{\zeta(3)}{N}\right)^{\frac{1}{3}} \frac{3}{2} \frac{\zeta(2)}{\zeta(3)} \left[\left(\frac{T}{T_c}\right)^2 \right. \\ & - \left(\frac{T}{T_c}\right)^3 \left. - \left(\frac{\zeta(3)}{N}\right)^{\frac{2}{3}} \frac{1}{\zeta(3)} \left\{ -\frac{3}{2} \frac{\zeta(2)^2}{\zeta(3)} \left[\left(\frac{T}{T_c}\right)^2 \right. \right. \right. \\ & - \left(\frac{T}{T_c}\right)^3 \left. \left. \left. + \left[\frac{T}{T_c} - \left(\frac{T}{T_c}\right)^3\right] \left[-\frac{1}{3} \ln\left(\frac{\zeta(3)}{N}\right) \right. \right. \right. \right. \\ & \left. \left. \left. + \gamma - \frac{19}{24} \right] + \frac{T}{T_c} \ln\left(\frac{T}{T_c}\right) \right\} + \dots \end{aligned} \quad (35)$$

Figure 4 shows how the approximation to describe a finite system with an order parameter deviates from the original grand-canonical approach without order parameter. In Figure 4a one observes in $D = 1$ dimension that the approximation introduced by the decomposition (11) is still noticeable at $T \approx T_c$ for $N = 10^4$ particles. For $D = 2$ dimensions, however, this effect becomes much smaller already for $N = 10^3$ particles as shown in Figure 4b. Note that equation (34) including the first finite-size correction yields a better agreement with the theory without order parameter than the already known leading order of (34).

4.3 Heat capacity

The heat capacity C_V can be found from (25) by using the relation $C_V = \partial U / \partial T\Big|_{V,N}$. One has to take into account two different regimes. For $T < T_c$ the chemical potential μ is fixed and the number of atoms in the ground state

N_0 depends on temperature. With this we get

$$C_{V,T \leq T_c} |_{D=1} = Nk_B \frac{2\zeta(2)}{\gamma - \ln(\hbar\omega\beta_c)} \frac{T}{T_c} + \dots, \quad (36)$$

$$C_{V,T \leq T_c} |_{D=2} = 2Nk_B \left(\frac{T}{T_c} \right)^2 \left\{ \frac{3\zeta(3)}{\zeta(2)} - \left(\frac{\zeta(3)}{N} \right)^{\frac{1}{2}} \right. \\ \left. \times \frac{3\zeta(3)}{\zeta(2)^2} \left[-\frac{1}{2} \ln \left(\frac{\zeta(2)}{N} \right) + \gamma - \frac{1}{2} \right] \right\} + \dots, \quad (37)$$

$$C_{V,T \leq T_c} |_{D=3} = 3Nk_B \left(\frac{T}{T_c} \right)^3 \left\{ \frac{4\zeta(4)}{\zeta(3)} \right. \\ \left. + \left(\frac{\zeta(3)}{N} \right)^{\frac{1}{3}} \left[\frac{3T_c}{T} - \frac{6\zeta(4)\zeta(2)}{\zeta(3)^2} \right] \right\} + \dots \quad (38)$$

For $T > T_c$, on the other hand, N_0 vanishes and μ depends on temperature. Thus, the heat capacity for $T > T_c$ still depends explicitly on T and μ . However, we can analytically work out the limit $T \downarrow T_c$ and obtain

$$\lim_{T \downarrow T_c} C_{V,T > T_c} |_{D=1} = Nk_B \frac{2\zeta(2)}{\gamma - \ln(\hbar\omega\beta_c)} + \dots, \quad (39)$$

$$\lim_{T \downarrow T_c} C_{V,T > T_c} |_{D=2} = 2Nk_B \\ \times \left(\frac{3\zeta(3)}{\zeta(2)} - \frac{2\zeta(2)}{1 + \gamma + \zeta(2) - \ln(\zeta(2)/N)/2} \right. \\ \left. + \left(\frac{\zeta(2)}{N} \right)^{\frac{1}{2}} \left\{ -\frac{3\zeta(3)}{\zeta(2)^2} \left[-\frac{1}{2} \ln \left(\frac{\zeta(2)}{N} \right) + \gamma - \frac{1}{2} \right] \right. \right. \\ \left. \left. + \frac{-\ln(\zeta(2)/N)/2 + 5/2 + 3\gamma - \ln 2 + 2\zeta(2)}{1 + \gamma + \zeta(2) - \ln(\zeta(2)/N)/2} \right. \right. \\ \left. \left. - \frac{-\ln(\zeta(2)/N)/2 + \gamma - 1/2 + \zeta(2)}{[1 + \gamma + \zeta(2) - \ln(\zeta(2)/N)/2]^2} \right\} \right) + \dots, \quad (40)$$

$$\lim_{T \downarrow T_c} C_{V,T > T_c} |_{D=3} = 3Nk_B \left(\frac{4\zeta(4)}{\zeta(3)} - 3 \frac{\zeta(3)}{\zeta(2)} + \left(\frac{\zeta(3)}{N} \right)^{\frac{1}{3}} \right. \\ \left. \times \left\{ \frac{3}{2} - 6 \frac{\zeta(4)\zeta(2)}{\zeta(3)^2} + \frac{3\zeta(3)}{\zeta(2)^2} \left[-\frac{1}{2} \ln \left(\frac{\zeta(3)}{N} \right) + \frac{5}{4} + \zeta(2) \right. \right. \right. \\ \left. \left. \left. + \frac{3}{2} \gamma \right] \right\} \right) + \dots \quad (41)$$

Thus, the heat capacity has a discontinuity at $T = T_c$ in $D = 2, 3$ which follows from (37), (38), (40), and (41):

$$\Delta C_V |_{D=2} = 2Nk_B \left\{ \frac{2\zeta(2)}{1 + \gamma + \zeta(2) - \ln(\zeta(2)/N)/2} \right. \\ \left. - \left(\frac{\zeta(2)}{N} \right)^{\frac{1}{2}} \left[-\frac{-\ln(\zeta(2)/N)/2 + \gamma - 1/2 + \zeta(2)}{[1 + \gamma + \zeta(2) - \ln(\zeta(2)/N)/2]^2} \right. \right. \\ \left. \left. + \frac{-\ln(\zeta(2)/N)/2 + 5/2 + 3\gamma - \ln 2 + 2\zeta(2)}{1 + \gamma + \zeta(2) - \ln(\zeta(2)/N)/2} \right] \right\} + \dots, \quad (42)$$

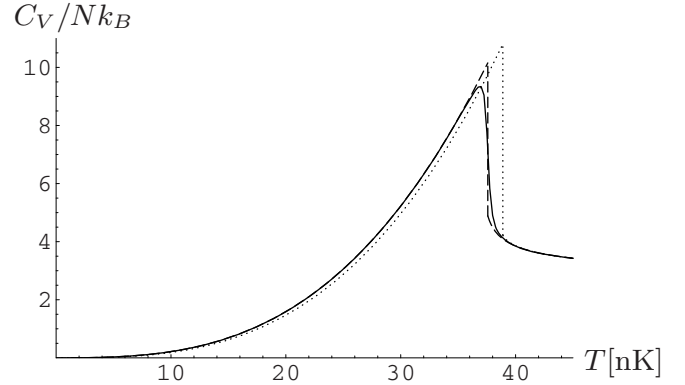


Fig. 5. Heat capacity C_V/Nk_B versus Temperature T in $D = 3$ dimensions for $\omega = 2\pi \cdot 40$ Hz and $N = 10^4$. The dotted (dashed) line is taken from equations (38), (41) and includes the leading order (the first two leading orders). The solid line corresponds to (8) from the theory without order parameter.

$$\Delta C_V |_{D=3} = 3Nk_B \left\{ \frac{3\zeta(3)}{\zeta(2)} - \left(\frac{\zeta(3)}{N} \right)^{\frac{1}{3}} \frac{3\zeta(3)}{\zeta(2)^2} \right. \\ \left. \times \left[-\frac{1}{2} \ln \left(\frac{\zeta(3)}{N} \right) + \frac{5}{4} + \zeta(2) + \frac{3}{2} \gamma - \frac{\zeta(2)^2}{2\zeta(3)} \right] \right\} + \dots \quad (43)$$

In $D = 3$ dimensions the discontinuity ΔC_V remains finite in the thermodynamic limit $N \rightarrow \infty$ and gets smaller for finite systems. This can be seen in Figure 5, where the heat capacity taken from (38) and (41) including the first finite-size correction are compared with the thermodynamic limit. In $D = 2$ dimensions one has a discontinuity for finite systems which vanishes in the thermodynamic limit $N \rightarrow \infty$. Finally, in $D = 1$ dimension there is no discontinuity ΔC_V at $T = T_c$ at all in leading order in agreement with the findings of reference [18]. Note that the leading contribution in the heat capacity discontinuities ΔC_V differs slightly from the findings in reference [18].

Note that equations (36)–(38) also provide systematic semiclassical expansions for both the internal energy U and the entropy S by using the thermodynamic relations $C_V = \partial U / \partial T |_{V,N} = T \partial S / \partial T |_{V,N}$ [24]. However, one does not need to work out the limit $T \rightarrow T_c$ separately above and below the critical point as both the internal energy U and the entropy S are continuous at $T = T_c$.

5 Conclusions

In this paper we have extended the usual semiclassical expansion [1,2,13,16] for harmonically confined ideal Bose gases. With this we have derived orders of the semiclassical expansion which have not yet been accessible using standard semiclassical approaches. This has been shown exemplarily for the critical temperature T_c as well as the temperature dependence of the condensate fraction N_0/N and the heat capacity C_V in $D = 1, 2, 3$ dimensions. It would be straight-forward to generalize our findings to anisotropic harmonic trapping potentials, which are used in many experiments to study Bose-Einstein condensation

in $D = 2, 3$. Finally, we note that it would be quite instructive to clarify the connection between our field-theoretic approach towards a systematic semiclassical expansion and the statistical approach of references [9,11,12,14,15] as both seem to be related (see the remark below Eq. (29)). However, this relation is by no means obvious as both the grand-canonical and the canonical approach rely on certain approximations.

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Appendix A: Semiclassical approximation

Some thermodynamic properties of the ideal Bose gas in a harmonic trap are expressible in terms of the series (23). Generalizing an approach of reference [23], Appendix 7A, we work out a systematic semiclassical approximation of (23) which is valid for $0 < b \ll 1$.

A.1 Euler-MacLaurin formula

In the limit of small b it is suggestive to approximate (23) by the Euler-MacLaurin formula

$$\sum_{k=0}^g f(k) = \int_0^g dk f(k) + \frac{f(0) + f(g)}{2} + \dots \quad (A.1)$$

However, this is not directly possible, as the integral would diverge if the series starts at $k = 0$. One way to avoid this divergency is to subtract all divergent terms in (23) before replacing the series by an integral. To this end we expand the denominator of (23) for small b

$$\frac{1}{(1 - e^{-bk})^D} = \sum_{l=0}^{D-1} \frac{C_l(D)}{(bk)^{D-l}} + \mathcal{O}(b^0), \quad (A.2)$$

where $C_0(D) = 1$, $C_1(D) = D/2$, $C_2(D) = D(3D-1)/24$, $C_3(D) = D^2(D-1)/48$, ... are the respective expansion coefficients. Afterwards we subtract this expansion from (23) and add it again:

$$I(A, b, D) = \sum_{k=0}^{\infty} e^{-bAk} \left[\frac{1}{(1 - e^{-bk})^D} - \sum_{l=0}^{D-1} \frac{C_l(D)}{(bk)^{D-l}} \right] + \sum_{k=1}^{\infty} \sum_{l=0}^{D-1} \frac{C_l(D) e^{-bAk}}{(bk)^{D-l}} + \mathcal{O}(b^0). \quad (A.3)$$

As we have extended the summation in the first line from $k = 1$ to $k = 0$, we have obtained an error of the order $\mathcal{O}(b^0)$. Finally, we apply (A.1) to the first line in (A.3),

where higher corrections can be neglected as they are as well of the order $\mathcal{O}(b^0)$. With this we arrive at

$$I(A, b, D) = \int_0^{\infty} dk e^{-bAk} \left[\frac{1}{(1 - e^{-bk})^D} - \sum_{l=0}^{D-1} \frac{C_l(D)}{(bk)^{D-l}} \right] + \sum_{k=1}^{\infty} \sum_{l=0}^{D-1} \frac{C_l(D) e^{-bAk}}{(bk)^{D-l}} + \mathcal{O}(b^0). \quad (A.4)$$

Both terms in (A.4) are treated as follows:

- We substitute $x = e^{-bk}$ in the first integral of (A.4). One immediately observes that the contribution of this integral is of the order $\mathcal{O}(b^{-1})$. Moreover one can re-express the first integral in terms of Gamma functions by using the Beta function ([31], Eq. (8.380))

$$B(x, y) = \int_0^1 dt t^{x-1} (1-t)^{y-1} = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}. \quad (A.5)$$

The remaining integrals in (A.4) can directly be evaluated using the integral representation of the Gamma function ([31], Eq. (8.310)):

$$\int_0^{\infty} dk k^{x-1} e^{-ka} = \frac{\Gamma(x)}{a^x}. \quad (A.6)$$

- The series in the second line of (A.4) can be expressed in terms of the polylogarithms (3).

With this we obtain eventually

$$I(A, b, D) = \frac{1}{b} \left[\frac{\Gamma(1-D)\Gamma(A)}{\Gamma(1+A-D)} - \sum_{l=0}^{D-1} C_l(D) \Gamma(1+l-D) \times A^{D-l-1} \right] + \sum_{l=0}^{D-1} \frac{C_l(D)}{b^{D-l}} \zeta_{D-l}(e^{-Ab}) + \mathcal{O}(b^0). \quad (A.7)$$

A.2 Dimensional regularisation

As the Gamma functions in (A.7) are divergent for integer dimension D , we apply dimensional regularization [32,33]. To this end we set $D = d - \epsilon$ with $d = 1, 2, 3, 4, \dots$ and consider the limit $\epsilon \rightarrow 0$. This leads to

$$I(A, b, d) = \lim_{\epsilon \rightarrow 0} \frac{1}{b} \left[\frac{\Gamma(1-d+\epsilon)\Gamma(A)}{\Gamma(1+A-d+\epsilon)} - \sum_{l=0}^{d-1} C_l(d-\epsilon) \Gamma(1+l-d+\epsilon) A^{d-l-1-\epsilon} \right] + \sum_{l=0}^{d-1} \frac{C_l(d)}{b^{d-l}} \zeta_{d-l}(e^{-Ab}) + \mathcal{O}(b^0). \quad (A.8)$$

In order to evaluate the limit $\epsilon \rightarrow 0$ we use the following expansion for the Gamma function

$$\Gamma(-n + \epsilon) = \frac{(-1)^n}{n!} \left\{ \frac{1}{\epsilon} + \psi_0(n+1) + \mathcal{O}(\epsilon^1) \right\} \quad (A.9)$$

with $n = 1, 2, 3, \dots$ and $\epsilon > 0$ ([32], Eq. (8D.24)). The digamma function $\psi_0(z)$ is defined as $\psi_0(z) = \Gamma'(z)/\Gamma(z)$. It satisfies the recursion formula ([32], Eq. (8D.6)) $\psi_0(z) = 1/(z-1) + \psi_0(z-1)$, where $\gamma = -\psi_0(1) = 0.5772\dots$ denotes Euler's constant. Moreover, we use the approximation $x^\epsilon = 1 + \epsilon \ln x + \dots$ and expand the coefficients $C_l(d-\epsilon) = C_l^{(0)}(d) - C_l^{(1)}(d)\epsilon + \mathcal{O}(\epsilon^2)$ for small ϵ , where $C_l^{(0)}(d) = C_l(d)$, $C_0^{(1)}(d) = 0$, $C_1^{(1)}(d) = 1/2$, $C_2^{(1)}(d) = (6d-1)/24$, $C_3^{(1)}(d) = d(3d-2)/48, \dots$ are the respective expansion coefficients. With this (A.8) reduces to

$$I(A, b, d) = \lim_{\epsilon \rightarrow 0} \frac{(-1)^{d-1}}{b} \left\{ \frac{1}{(d-1)!} \left[\prod_{l=1}^{d-1} (A-l) \right] \right. \\ \times \left[\frac{1}{\epsilon} - \psi_0(1+A-d) + \psi_0(d) \right] \sum_{l=0}^{d-1} \frac{(-1)^l C_l^{(0)}(d)}{(d-l-1)!} \\ \times \left[\frac{1}{\epsilon} + \psi_0(d-l) - \frac{C_l^{(1)}(d)}{C_l^{(0)}(d)} - \ln(A) \right] A^{d-l-1} \left. \right\} \\ + \sum_{l=0}^{d-1} \frac{C_l^{(0)}(d)}{b^{d-l}} \zeta_{d-l}(e^{-Ab}) + \mathcal{O}(b^0). \quad (\text{A.10})$$

Equation (A.10) can be further simplified if one uses the identity

$$\frac{1}{(d-1)!} \prod_{l=1}^{d-1} (A-l) = \sum_{l=0}^{d-1} \frac{(-1)^l C_l^{(0)}(d)}{(d-l-1)!} A^{d-l-1}, \quad (\text{A.11})$$

which can be proven by complete induction. Thus, the terms in (A.10), which are proportional to $1/\epsilon$, cancel and we obtain a finite result in the limit $\epsilon \rightarrow 0$. Using the recursion formula of the digamma function one arrives at

$$I(A, b, d) = \frac{1}{b} \sum_{l=0}^{d-1} \frac{(-1)^{d-l-1} C_l^{(0)}(d)}{(d-l-1)!} A^{d-l-1} \\ \times \left[-\psi_0(1+A-d) + \ln A + \frac{C_l^{(1)}(d)}{C_l^{(0)}(d)} + \sum_{m=d-l}^{d-1} \frac{1}{m} \right] \\ + \sum_{l=0}^{d-1} \frac{C_l^{(0)}(d)}{b^{d-l}} \zeta_{d-l}(e^{-Ab}) + \mathcal{O}(b^0). \quad (\text{A.12})$$

Assuming $0 < b \ll 1$ we read off that equation (A.12) is, indeed, a good approximation for (23) as the error is of the order $\mathcal{O}(b^0)$. For different dimensions $d = 1, 2, 3, 4$ one

gets explicitly

$$I(A, b, 1) = \frac{1}{b} [\ln A - \psi_0(A) + \zeta_1(e^{-Ab})] + \mathcal{O}(b^0), \quad (\text{A.13})$$

$$I(A, b, 2) = \frac{1}{b^2} \zeta_2(e^{-Ab}) + \frac{1}{b} \left\{ -(A-1) [\ln A - \psi_0(A-1)] \right. \\ \left. + \frac{3}{2} + \zeta_1(e^{-Ab}) \right\} + \mathcal{O}(b^0), \quad (\text{A.14})$$

$$I(A, b, 3) = \frac{1}{b^3} \zeta_3(e^{-Ab}) + \frac{3}{2b^2} \zeta_2(e^{-Ab}) + \frac{1}{b} \left\{ \frac{1}{2}(A-1) \right. \\ \times (A-2) [\ln A - \psi_0(A-2)] - \frac{5}{4}A + \frac{53}{24} \\ \left. + \zeta_1(e^{-Ab}) \right\} + \mathcal{O}(b^0), \quad (\text{A.15})$$

$$I(A, b, 4) = \frac{1}{b^4} \zeta_4(e^{-Ab}) + \frac{2}{b^3} \zeta_3(e^{-Ab}) + \frac{11}{6b^2} \zeta_2(e^{-Ab}) \\ + \frac{1}{b} \left\{ + \frac{7}{12}A^2 - \frac{179}{72}A + \frac{8}{3} + \zeta_1(e^{-Ab}) - \frac{1}{6}(A-1) \right. \\ \left. \times (A-2)(A-3) [\ln A - \psi_0(A-3)] \right\} + \mathcal{O}(b^0). \quad (\text{A.16})$$

Note that the respective polylogarithmic functions in (A.13)–(A.16) have to be evaluated for small b by using the Robinson formula (26).

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