Bose–Einstein condensation temperature of finite systems

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Abstract. In studies of the Bose–Einstein condensation of ideal gases in finite systems, the divergence problem usually arises in the equation of state. In this paper, we present a technique based on the heat kernel expansion and zeta function regularization to solve the divergence problem, and obtain the analytical expression of the Bose–Einstein condensation temperature for general finite systems. The result is represented by the heat kernel coefficients, where the asymptotic energy spectrum of the system is used. Besides the general case, for systems with exact spectra, e.g. ideal gases in an infinite slab or in a three-sphere, the sums of the spectra can be obtained exactly and the calculation of corrections to the critical temperatures is more direct. For a system confined in a bounded potential, the form of the heat kernel is different from the usual heat kernel expansion. We show that as long as the asymptotic form of the global heat kernel can be found, our method works. For Bose gases confined in three- and two-dimensional isotropic harmonic potentials, we obtain the higher-order corrections to the usual results of the critical temperatures. Our method can also be applied to the problem of generalized condensation, and we give the correction of the boundary on the second critical temperature in a highly anisotropic slab.

Keywords: Bose–Einstein condensation, cold atoms
1. Introduction

Since the experimental realization of Bose–Einstein condensation (BEC) in ultracold atoms [1–3], numerous theoretical studies have devoted attention to the BEC phase transition in finite systems. Strictly speaking, a phase transition can only occur in infinite systems. In a finite system, all thermodynamic quantities are analytical functions of the temperature, so there is no genuine phase transition. On the other hand, the behavior of a large system is practically the same as that of an infinite one just as observed in experiments, so a (quasi-)critical temperature is needed to discuss the properties of finite systems. To define the critical temperature of BEC in a finite system, many schemes with different criteria have been discussed, such as those that use a small value of the condensate fraction [4–7], the maximal fluctuation or inflexion point of the ground-state occupation number [8], the maximum of the specific heat [9, 10], etc.

The heat kernel approach [11–13] is a powerful tool for studying the BEC phase transition. In the past few years, the heat kernel approach has been widely applied in many fields of physics, including quantum field theory [14–16], quantum gravity [17, 18], string theory [19], and quantum statistical mechanics [11, 20]. However, when applied to the BEC of an ideal gas in a finite system, the heat kernel expansion encounters the problem of divergence. In fact, the problem of divergence is also inevitable in approaches other than the heat kernel expansion. If one regards that the phase transition occurs at the chemical potential $\mu = 0$ just as that in the thermodynamic
limit, the equation of state of the gas is divergent \[5, 7, 21\]. To avoid this difficulty, discussion of the phase transition in finite systems usually ignores the divergent terms \[4, 9–11, 22, 23\] or, for systems with exact energy spectra, directly obtains the sum of the spectra \[5, 24, 25\].

In this paper, we present a technique for solving the divergence problem in the BEC phase transition of nonrelativistic ideal gases confined in finite systems, with the help of the heat kernel expansion and zeta function regularization. By using the asymptotic spectrum calculated from the heat kernel expansion, we obtain the analytical expression of the critical temperature for ideal Bose gases in general finite systems, which is expressed only by the heat kernel coefficients. In this result, the effect of the finite number of particles is separated from other factors. We compare it with the numerical result of the specific heat of an ideal Bose gas in a cube with period boundary conditions, and they fit very well. Our result also shows the influence of the boundary on the critical temperature for an arbitrary cavity. Furthermore, when the sum of the energy spectra can be exactly obtained, we can replace the asymptotic result with the exact sum and obtain a more precise critical temperature. The critical temperatures of BEC in an infinite slab and in a three-sphere \(S^3\) are given as examples, and the results are consistent with those calculated by other methods. In a bounded potential, the heat kernel has a different form from the usual heat kernel expansion. Our method can also be applied to such cases. As examples, we give the higher-order corrections to the critical temperatures of BEC in three- and two-dimensional isotropic harmonic potentials. In addition, in highly anisotropic systems the condensation may not occur in the ground state but is distributed in a set of single-particle states, i.e. generalized BEC \[26–28\]. Bose gases in such systems may undergo two kinds of phase transitions. We also consider the influence of the boundary on the second critical temperature in a highly anisotropic slab.

The paper is organized as follows. In section 2, we discuss the BEC phase transition of an ideal gas in a general finite system and express the critical temperature analytically in terms of the heat kernel coefficients. As examples, we discuss the influence of the finite number of particles and the boundary. In section 3, we calculate the critical temperatures of BEC in an infinite slab and in a three-sphere. In these cases the sums of the energy spectra are exactly obtained. In section 4, we consider the phase transition in three- and two-dimensional isotropic harmonic traps, and obtain the higher-order corrections to the critical temperatures. In section 5, we discuss the correction of the boundary on the second critical temperature in a highly anisotropic slab. Conclusions and some points of discussion are presented in section 6.

2. Critical temperature of BEC in finite systems

In the grand canonical ensemble, the grand potential of an ideal Bose gas is

\[
\ln \Xi = - \sum_i \ln \left( 1 - ze^{-\beta E_i} \right),
\]
where \( \{E_i\} \) is the single-particle energy spectrum, the fugacity \( z = e^{\beta \mu} \) with \( \mu \) denoting the chemical potential, and \( \beta = 1/(k_B T) \) with \( k_B \) denoting the Boltzmann constant. Expanding the logarithmic term gives

\[
\ln \Xi = \sum_{\ell=1}^{\infty} \frac{1}{\ell} z^\ell \sum_i e^{-\ell \beta E_i}.
\] (2)

Since the energy spectrum satisfies the eigenvalue equation

\[
\left[-\nabla^2 + \frac{2m}{\hbar^2} V(x)\right] \psi_i = \frac{2m}{\hbar^2} E_i \psi_i,
\] (3)

the sum over the spectrum in equation (2) can be expressed as the global heat kernel of the operator \( D = -\nabla^2 + \left(2m/\hbar^2\right) V(x) \). Mathematically, the global heat kernel of an operator \( D \) is defined as

\[
K(t) = \sum_i e^{-\lambda_i t},
\] (4)

where \( \{\lambda_i\} \) is the spectrum of the operator \( D \). When \( t \to 0 \), it can be asymptotically expanded as a series of \( t \), which is the heat kernel expansion,

\[
K(t) \approx \frac{1}{(4\pi t)^{3/2}} \sum_{k=0, \frac{1}{2}, 1, \ldots} B_k t^k, \quad (t \to 0)
\] (5)

where \( B_k \ (k = 0, 1/2, 1, \ldots) \) denotes the heat kernel coefficients. Therefore, with the help of the heat kernel expansion, the grand potential in equation (2) can be rewritten as

\[
\ln \Xi = \sum_{\ell=1}^{\infty} \frac{1}{\ell} K\left(t \frac{\hbar^2 \beta}{2m}\right) z^\ell = \frac{1}{\lambda^3} \sum_{k=0, \frac{1}{2}, 1, \ldots} \frac{B_k}{(4\pi)^k} \lambda^{2k} g_{k/2-k} (z),
\] (6)

where

\[
g_\sigma (z) = \frac{1}{\Gamma(\sigma)} \int_0^\infty \frac{x^{\sigma-1}}{z^{\sigma-1}e^x-1} dx = \sum_{k=1}^{\infty} \frac{z^k}{k^{\sigma}}
\] (7)

is the Bose–Einstein integral, and \( \lambda = \sqrt{2\pi \beta \hbar / \sqrt{m}} \) is the mean thermal wavelength. For a system with a fixed number of particles, the relation between the fugacity \( z \) and the temperature \( T \) is given by the equation of the particle number

\[
N = \left(z \frac{\partial \ln \Xi}{\partial z}\right)_{V, T} = \frac{1}{\lambda^3} \sum_{k=0, \frac{1}{2}, 1, \ldots} \frac{B_k}{(4\pi)^k} \lambda^{2k} g_{k/2-k} (z),
\] (8)

or,

\[
n \lambda^3 = g_{3/2} (z) + \frac{B_{1/2}}{4\pi V} \lambda g_1 (z) + \frac{B_1}{4\pi V} \lambda^2 g_{1/2} (z) + \cdots,
\] (9)

where \( n = N/V \) is the particle number density, and we take \( B_0 = V \).
Clearly, the first terms in equations (6) and (9) give the ordinary equation of state for an ideal Bose gas in the thermodynamic limit. The other terms in these equations describe the difference between a finite system and that in the thermodynamic limit. To discuss the BEC phase transition in the thermodynamic limit, one only needs to set \( z = 1 \) or the chemical potential \( \mu = 0 \) in the equation of the particle number, and then the critical temperature can be obtained immediately. However, since the Bose–Einstein integral \( g_\sigma (1) \) is divergent at \( \sigma \leq 1 \), the correction terms in equation (9) become singular at \( \mu = 0 \). In other words, the traditional method for determining the critical temperature is invalid for the system described by equation (9).

In the following, we show that, based on the heat kernel expansion and zeta function regularization, we can solve the divergence problem and obtain an analytical expression of the critical temperature of BEC.

At the transition point, the chemical potential \( \mu \to 0 \), and the leading term of the asymptotic expression of the Bose–Einstein integral is

\[
g_\sigma (e^{\beta \mu}) \approx \begin{cases} 
\zeta (\sigma), & (\sigma > \frac{3}{2}) \\
- \ln (\beta \mu), & (\sigma = 1) \\
\Gamma (-\sigma + 1) \frac{1}{(\beta \mu)^{1/2}}, & (\sigma \leq \frac{1}{2}) 
\end{cases} (\mu \to 0)
\]

where \( \zeta (\sigma) = \sum_{n=1}^{\infty} n^{-\sigma} \) is the Riemann zeta function. Expanding equation (9) and keeping the leading term of the Bose–Einstein integrals, we reach its asymptotic expression for \( \mu \to 0 \):

\[
n\lambda^3 \approx \zeta \left( \frac{3}{2} \right) - \frac{B_{1/2}}{\sqrt{4\pi V}} \lambda \ln (\beta \mu) + I,
\]

where

\[
I = \sum_{k=1, \frac{3}{2}, 2, \cdots} B_k \frac{\lambda^{2k}}{(4\pi)^k V^{2k}} \Gamma \left( k - \frac{1}{2} \right) \frac{1}{(\beta \mu)^{k-1/2}}
\]

is introduced for simplicity. When \( \mu \to 0 \), this is a series in which every term is divergent. However, it can be summed up by use of the heat kernel expansion and equation (11) will give an analytical result. We describe the procedure in the following.

First, we represent the gamma function in equation (12) as an integral and introduce a small regularization parameter \( s \) to deal with the divergence problem, i.e.

\[
\Gamma (\xi) = \int_0^\infty x^{\xi-1+se^{-x}} dx \quad (s \to 0).
\]

Then equation (12) becomes

\[
I = \frac{\sqrt{\beta \mu}}{V} \int_0^\infty dx x^{s-3/2} e^{-x} \sum_{k=1, \frac{3}{2}, 2, \cdots} B_k \left( \frac{\hbar^2}{2m} - \mu \right)^k.
\]

The sum in the integral differs from the heat kernel expansion equation (5) just by two extra terms and a common coefficient, so we can express equation (14) by the global heat kernel as
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\[ I = \frac{\sqrt{-\beta \mu}}{V} \int_0^\infty dx x^{s-3/2} e^{-x} \left[ \left( \frac{\hbar^2}{4\pi} \frac{x}{2m-\mu} \right)^{3/2} K \left( \frac{\hbar^2}{2m-\mu} \right) \right] \]

\[ = \frac{\lambda^3}{V - \beta \mu} \int_0^\infty dx x^{s} e^{-x} K \left( \frac{\hbar^2}{2m-\mu} \right) - \Gamma \left( s - \frac{1}{2} \right) \sqrt{-\beta \mu} - \Gamma (s) \frac{B_{1/2} \lambda}{\sqrt{4\pi V}}. \]  

(15)

As a result, the divergent sum in equation (12) is converted to the global heat kernel.

Next, the integral in the first term in equation (15) can be obtained by substituting the definition of the global heat kernel equation (4),

\[ \int_0^\infty dx x^{s} e^{-x} K \left( \frac{\hbar^2}{2m-\mu} \right) = \sum_{i=1}^\infty \int_0^\infty dx x^{s} e^{-E_i} = \Gamma (1 + s) \sum_{i=1}^\infty \frac{(-\mu)^{1+s}}{(E_i - \mu)^{1+s}}. \]  

(16)

Our aim is to determine the critical temperature of the BEC, which occurs at \( \mu \to 0 \). At this limit, equation (15) becomes

\[ I = \Gamma (1 + s) \frac{\lambda^3}{V} \frac{(-\mu)^s}{\beta} \sum_{i=1}^\infty \frac{1}{E_i^{1+s}} - \Gamma (s) \frac{B_{1/2} \lambda}{\sqrt{4\pi V}}. \]  

(17)

Note that the sum of the spectrum is indeed the spectrum zeta function defined as \( \zeta_s (\sigma) = \sum_{i=1}^\infty \lambda_i^{-\sigma} \), which gives

\[ \sum_{i=1}^\infty \frac{1}{E_i^{1+s}} = \left( \frac{2m}{\hbar^2} \right)^{1+s} \sum_{i=1}^\infty \frac{1}{\lambda_i^{1+s}} = \left( \frac{2m}{\hbar^2} \right)^{1+s} \zeta_s (1 + s). \]  

(18)

Equation (11) now is

\[ n \lambda^3 = \zeta \left( \frac{3}{2} \right) \frac{B_{1/2} \lambda}{\sqrt{4\pi V}} \ln (-\beta \mu) + \Gamma (1 + s) \frac{\lambda^3}{V} \frac{(-\mu)^s}{\beta} \sum_{i=1}^\infty \frac{1}{E_i^{1+s}} - \Gamma (s) \frac{B_{1/2} \lambda}{\sqrt{4\pi V}}. \]  

(19)

Although this result is based on the whole heat kernel expansion, only the first two heat kernel coefficients \( B_0 = V \) and \( B_{1/2} \) appear in this expression. However, it does not mean that the higher-order heat kernel coefficients are irrelevant to the critical temperature. In equation (19), there is a term for the sum of the spectrum, and information on the spectrum is embodied in the heat kernel coefficients.

Finally, we deal with the sum in equation (19). For a general system, the exact spectrum is not known, but we can obtain its asymptotic expression on the basis of the heat kernel expansion. As given in [29], we can first obtain the counting function from the heat kernel expansion, and then achieve the asymptotic expansion of the spectrum from the counting function. Specifically, the counting function \( N (\chi) \) is defined as the number of eigenstates of an operator with the eigenvalue smaller than \( \chi \). The relation between the counting function and the global heat kernel is [29]

\[ N (\chi) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} K (t) \frac{e^{\chi t}}{t} dt. \]  

(20)

From the heat kernel expansion equation (5), we can calculate the asymptotic expansion of the counting function.
The energy spectrum $E_i = (\hbar^2/2m) \lambda_i$, according to equation (23) we have

$$\sum_{i=1}^{\infty} \frac{1}{E_i^{1+s}} \approx \sum_{i=1}^{\infty} \left[ \frac{2m}{\hbar^2} \frac{B_0}{6 \pi^2} \right]^{2/3} \left[ 1 + \frac{(1 + s) B_{1/2}}{2 \cdot 6^{1/3} \pi^{1/6} B_0^{1/3} \lambda^{1+2s/3}} \right]^{1+s} \left[ \zeta \left( \frac{2}{3} \right) + \frac{2s}{3} \right] + \frac{(1 + s) B_{1/2}}{2 \cdot 6^{1/3} \pi^{1/6} V^{2/3}} \zeta \left( 1 + \frac{2s}{3} \right) \right]. \quad (24)$$

In this calculation, we represent the sum by the Riemann zeta function. Note that by zeta function regularization, the two divergent sums are replaced by zeta functions. However, the second term in equation (24) still contains a function $\zeta \left( 1 + \frac{2s}{3} \right)$ which is divergent as $s \to 0$. Substituting this result into equation (17) and expanding it around $s = 0$ gives

$$I \approx \frac{4 \zeta (2/3) \lambda}{6^{2/3} \pi^{1/3} V^{1/3}} - \frac{B_{1/2}}{\sqrt{4 \pi V}} \left( \ln \frac{3^{2/3} \pi^{4/3} \hbar^2}{2^{1/3} m V^{2/3}} - \ln \frac{3^{2/3} \pi^{1/3} \lambda^2}{2^{4/3} V^{2/3}} - 1 - \gamma_E \right), \quad (25)$$

where $\gamma_E = 0.5772$ is the Euler constant. We find that the linearly divergent terms of $s$ from the zeta function and the gamma function have been canceled. On the other hand, there is a logarithmically divergent term of $\mu$ in this equation, but this term is also canceled when substituting equation (25) into (11):

$$n \lambda^3 = \zeta \left( \frac{3}{2} \right) + \frac{4 \zeta (2/3) \lambda}{6^{2/3} \pi^{1/3} V^{1/3}} - \frac{B_{1/2} \lambda}{\sqrt{4 \pi V}} \left( \ln \frac{3^{2/3} \pi^{4/3} \hbar^2}{2^{1/3} m V^{2/3}} - \ln \frac{3^{2/3} \pi^{1/3} \lambda^2}{2^{4/3} V^{2/3}} - 1 - \gamma_E \right). \quad (26)$$

With the above technique, our final equation (26) is fully analytical now. This equation holds at the transition point, so the critical temperature can be solved straightforwardly. Clearly, the first term on the right-hand side of equation (26) gives the critical temperature in the thermodynamic limit:

$$T_0 = \frac{2 \pi \hbar^2 n^{2/3}}{\zeta^{2/3} (3/2) m k_B}. \quad (27)$$

Regarding the last two terms in equation (26) as small corrections, we can obtain the critical temperature $T_c$, satisfying
This result shows that the correction to the critical temperature of an ideal Bose gas in a finite system is represented by the heat kernel coefficients. Since the typical case of nonvanishing $B_{1/2}$ is a system with a boundary, one direct application of this result is the description of the influence of the boundary on the critical temperature. Besides, the first term in equation (28) is proportional to $1/N^{1/3}$, or it is only related to the particle number. This indicates that this term describes the pure contribution of the finite number of particles.

Equation (28) only contains two terms since we only consider the first two terms in the asymptotic expression of the spectrum equation (23). More contributions can be easily obtained by including more terms in equation (23), and each of them will yield a term proportional to some $\zeta(\alpha)$ with $\alpha > 1$, so there is no divergence in these terms and the calculation is straightforward. It is easy to check that all these contributions are also proportional to $1/N^{1/3}$.

In the following, we consider two examples to show the correction in equation (28) to the critical temperature.

### 2.1. Effect of the finite number of particles

According to equation (28), if the only influence on the ideal gas is the finite number of particles, the critical temperature of the BEC is

$$\frac{T_c - T_0}{T_0} \approx \frac{2}{9\zeta^{2/3}(3/2)} \left[ -\frac{3^{1/3}4^{2/3}\zeta(2/3)}{\pi^{1/3}} - \frac{1}{\sqrt{\pi}} \left( \ln \frac{4N}{3\sqrt{\pi} \zeta(3/2)} + \frac{3}{2} + \gamma_E \right) B_{1/2} \right] \frac{1}{V^{2/3}} \approx 0.7115 \frac{1}{N^{1/3}}. \quad (29)$$

Therefore, the critical temperature increases in a finite system compared with that in the thermodynamic limit.

To check this result, we consider an ideal Bose gas confined in a three-dimensional cube of side length $L$ with period boundary conditions. The single-particle energy spectrum is

$$E(n_x, n_y, n_z) = \frac{2\pi^2\hbar^2}{mL^2} \left( n_x^2 + n_y^2 + n_z^2 \right). \quad (n_x, n_y, n_z = 0, \pm 1, \pm 2, \cdots). \quad (30)$$

The corresponding global heat kernel can be obtained by repeatedly applying the Euler–MacLaurin formula [30]:

$$K\left(\frac{\hbar^2\beta}{2m}\right) = \sum_{n_x, n_y, n_z = -\infty}^{\infty} e^{-\beta E(n_x, n_y, n_z)} \approx \left( \frac{2\pi\hbar^2\beta}{m} \right)^{-3/2} V. \quad (31)$$

The heat kernel expansion only contains one term just like that in infinite space, but it is not an exact result since some exponentially small terms have been neglected. This form implies that the only factor affecting the critical temperature in such a system is the volume, or the particle number. In other words, the critical temperature of BEC in this system should satisfy equation (29).

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In figure 1 we plot the exact numerical result of the specific heat versus the temperature for an ideal Bose gas in the cube with period boundary conditions. The critical temperature given by equation (29) agrees very well with the maximum of the specific heat.

2.2. Effect of the boundary

The influence of the boundary on BEC with different boundary conditions has motivated many studies [31–33]. In the following, we discuss the influence of the boundary on the critical temperature according to equation (28). We know that at a manifold with a boundary, the coefficient $B_{1/2}$ reflects the leading effect of the boundary [12]

$$B_{1/2} = \mp \frac{\sqrt{\pi}}{2} S,$$  \hspace{1cm} (32)

where $S$ is the surface area of the system, and the signs $-$ and $+$ correspond to the Dirichlet and Neumann boundary conditions, respectively. Substituting equation (32) into (28) gives the critical temperature for the corresponding system.

To check the result, we consider a Bose gas confined in a cube of side length $L$ with Dirichlet boundary conditions. The energy spectrum is

$$E(n_x, n_y, n_z) = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2), \quad (n_x, n_y, n_z = 1, 2, 3, \cdots)$$  \hspace{1cm} (33)

and the heat kernel coefficients are [29]

$$B_0 = L^3, B_{1/2} = -3\sqrt{\pi}L^2, B_1 = 3\pi L,$$

$$B_{3/2} = -\pi^{3/2}, B_k = 0 \left( k > \frac{3}{2} \right).$$  \hspace{1cm} (34)

Then, according to equation (28), the correction to the critical temperature is

$$\frac{T_c - T_0}{T_0} = \frac{2}{3\zeta^{2/3}(3/2)} \left[ -\frac{4^{2/3}\zeta(2/3)}{3^{2/3}\pi^{1/3}} + \left( \ln \frac{4N}{3\sqrt{\pi} \zeta(3/2)} + \frac{3}{2} + \gamma_E \right) \right] \frac{1}{N^{1/3}}$$

$$= (0.3515 \ln N + 1.004) \frac{1}{N^{1/3}}.$$

Clearly, this result contains the contributions from the finite number of particles and the boundary. As mentioned above, in equation (35) only the first-order correction of the spectrum is included. If more terms are included in the asymptotic expansion of the spectrum equation (23), we can obtain a more precise critical temperature. The final result converges to

$$\frac{T_c - T_0}{T_0} = (0.3515 \ln N + 0.257) \frac{1}{N^{1/3}}.$$  \hspace{1cm} (36)

The $\ln N$ term in the parentheses is consistent with [31].

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3. Systems with exact spectra

In section 2, we give a general discussion on the critical temperature of BEC, in which the asymptotic expansion of the spectrum equation (23) is taken into account. However, if the spectrum of the system is known and can be summed exactly, we can obtain the sum and a more precise critical temperature. In the following we consider two examples: an infinite slab and a three-sphere $S^3$.

3.1. BEC in an infinite slab

Consider a Bose gas between two infinite parallel planes with distance $L$. It can be regarded as a rectangular box of side lengths $L_x = L_y = a$ ($a \to \infty$) and $L_z = L$ with Dirichlet boundary conditions. The single-particle energy spectrum then is

$$E(n_x, n_y, n_z) = \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_x^2}{a^2} + \frac{n_y^2}{a^2} + \frac{n_z^2}{L^2} \right). \quad (n_x, n_y, n_z = 1, 2, 3, \cdots).$$

(37)

For such a form of the spectrum, the sum in equation (18) can be obtained exactly. Since $a \to \infty$, the sums of $n_x$ and $n_y$ are converted to integrals, and we have

$$\sum_{n_x, n_y, n_z=1}^{\infty} \frac{1}{E(n_x, n_y, n_z)^{1+s}} = \left( \frac{\pi^2 \hbar^2}{2m} \right)^{-(1+s)} \sum_{n_z=1}^{\infty} \int_0^{\infty} dn_x dn_y \frac{1}{\left( \frac{n_x^2}{a^2} + \frac{n_y^2}{a^2} + \frac{n_z^2}{L^2} \right)^{1+s}}$$

$$= \left( \frac{\pi^2 \hbar^2}{2m} \right)^{-(1+s)} \sum_{n_z=1}^{\infty} \frac{\pi a^2}{4s} \left( \frac{n_z^2}{L^2} \right)^{-s} = \left( \frac{\pi^2 \hbar^2}{2m} \right)^{-(1+s)} \pi a^2 L^{2s} \frac{1}{4s} \zeta(2s) \frac{1}{s}. \quad (38)$$

Figure 1. The numerical result of the specific heat versus the temperature for an ideal Bose gas in a cube with period boundary conditions. The three curves represent the cases with the particle number $N = 10^3$ (black solid line), $N = 10^4$ (red dotted line), and $N = 10^5$ (blue dashed line), respectively. The critical temperatures given by equation (29) for these cases are represented by the vertical dashed lines.
The heat kernel coefficients for the Laplace operator can also be calculated from the spectrum equation (37),

\[ B_0 = V = a^2L, \ B_{1/2} = -\sqrt{\pi}a^2, \ B_k = 0 \quad (k > \frac{1}{2}). \]  

(39)

At the transition point, \( \mu \to 0 \), equation (19) becomes

\[ n\lambda^3 = \zeta \left( \frac{3}{2} \right) + \frac{\lambda}{2L} \ln (-\beta \mu) + \frac{\lambda}{L^{1-2s}} \left( -\frac{2m\mu}{\pi^2\hbar^2} \right)^s \Gamma (1 + s) \zeta (2s) \frac{1}{s} + \frac{\lambda}{2L} \Gamma (s). \]  

(40)

When \( s \to 0 \), all of the divergent terms in this expression are canceled, and we have

\[ n\lambda^3 = \zeta \left( \frac{3}{2} \right) + \frac{\lambda}{2L} \ln \left( \frac{\lambda^2}{16\pi L^2} \right). \]  

(41)

This equation holds at the transition point. The second term represents the correction from the boundary. Then we can obtain the correction to the critical temperature:

\[ \frac{T_c - T_0}{T_0} \approx \frac{1}{3\zeta^{2/3} (3/2)} \ln \left( \frac{16\pi}{\zeta^{2/3} (3/2) n^{2/3} L^2} \right) \frac{1}{n^{1/3} L} = \left[ 0.3514 \ln (n^{1/3} L) + 0.5758 \right] \frac{1}{n^{1/3} L}. \]  

(42)

This result is consistent with that in [24], in which the critical temperature is obtained by use of the Mellin–Barnes transform.

3.2. BEC in the three-sphere

The spectrum of the Laplace operator in a three-sphere \( S^3 \) of radius \( R \) is [34]

\[ \lambda_n = n (n + 2) \frac{1}{R^2} \]  

(43)

with a degeneracy of \((n + 1)^2\). The global heat kernel is [35]

\[ K (t) = \frac{V}{(4\pi t)^{3/2}} e^{-\frac{t}{4}}. \]  

(44)

where \( V = 2\pi^2 R^3 \) is the volume of \( S^3 \). Therefore, the heat kernel expansion in \( S^3 \) does not contain half-integer powers of \( t \). In fact, this result can be obtained directly without the specific form of the heat kernel: Since \( S^3 \) is a smooth manifold without boundaries, the heat kernel expansion will not contain half-integer power terms.

According to the analysis in section 2, the critical temperature satisfies equation (19). For the \( S^3 \) case, the coefficient \( B_{1/2} = 0 \), which makes the divergent terms in the general case vanish, so we can take \( s = 0 \) in the expression, i.e.

\[ n\lambda^3 = \zeta \left( \frac{3}{2} \right) + \frac{\lambda^3}{V \beta} \sum_{i=1}^{\infty} \frac{1}{E_i}. \]  

(45)

Then we obtain the sum by using the exact spectrum equation (43). The sum of all the excited states is
\[
\sum_{i=1}^{\infty} \frac{1}{E_i} = \frac{2mR^2}{\hbar^2} \sum_{n=1}^{\infty} \frac{(n+1)^2}{n(n+2)} = \frac{2mR^2}{\hbar^2} \sum_{n=2}^{\infty} \frac{n^2}{n^2 - 1}
\]
\[
= \frac{2mR^2}{\hbar^2} \sum_{n=2}^{\infty} \sum_{k=0}^{n} n^{-2k} = \frac{2mR^2}{\hbar^2} \sum_{k=0}^{\infty} (\zeta(2k) - 1)
\]
\[
= -\frac{3mR^2}{2\hbar^2}, \tag{46}
\]

where we use equation (215) in [36]
\[
\sum_{k=1}^{\infty} (\zeta(2k) - 1) = \frac{3}{4}. \tag{47}
\]

Then equation (45) becomes
\[
n\lambda^3 = \zeta\left(\frac{3}{2}\right) - \frac{3}{2^{2/3} \pi^{1/3} \sqrt[3]{1}} \lambda \tag{48}
\]

and the correction to the critical temperature is
\[
\frac{T_c - T_0}{T_0} \approx \frac{2^{1/3}}{\pi^{1/3} \zeta^{2/3} (\frac{3}{2})^{4/3}} \frac{1}{N^{1/3}} = 0.4535 \frac{1}{N^{1/3}} \tag{49}
\]

In [24], the authors also discuss BEC in $S^3$. Their result has a different coefficient from equation (49), but the reason is that the spectrum in [24] is approximated as $\lambda_n = (n+1)^2/R^2$. If we use this spectrum too, our result will be the same as that in [24].

4. BEC in harmonic potentials

In section 2, our discussion is based on the heat kernel expansion equation (5). However, if an ideal Bose gas is confined in a bounded potential, the form of the heat kernel changes. In this section, we show that even if the form of the heat kernel is different from equation (5), the above method can still be used to determine the critical temperature of BEC. We take three- and two-dimensional harmonic potentials as examples.

4.1. Three-dimensional harmonic potentials

In the literature, many studies devote attention to the BEC phase transition in three-dimensional harmonic potentials since the BEC of ultracold atoms is realized in such potentials. In a harmonic potential, the heat kernel of the Laplace operator has a different form from equation (5), but it still can be expanded as a series. At the transition point, one also encounters the problem of divergence. In many theoretical studies on the critical temperature of BEC in harmonic potentials based on the heat kernel approach, the divergent terms are ignored [4, 9, 10, 23]. In this section, we apply the technique provided in section 2 to consider all the terms in the equation of state. By
solving the divergence problem, we obtain the analytical result for the critical temperature with higher-order correction.

The energy spectrum of a particle in a three-dimensional isotropic harmonic potential is

$$E_n = n\hbar\omega$$  \hspace{1cm} (50)

with the degenerate degree $$(n + 1)(n + 2)/2$$, where the zero-point energy is suppressed. Then the heat kernel is

$$K(t) = \sum_{n=0}^{\infty} \frac{1}{2}(n + 1)(n + 2)e^{-nt} = \frac{1}{(1 - e^{-t})^3} = \sum_{k=0}^{\infty} C_k t^{k-3},$$  \hspace{1cm} (51)

where the coefficients are

$$C_0 = 1, C_1 = \frac{3}{2}, C_2 = 1, \ldots.$$  \hspace{1cm} (52)

Although the form of the heat kernel expansion is different from equation (5), we can apply the same procedure to discuss the BEC phase transition in the harmonic potential.

Replacing equation (5) with (51) and substituting it into the grand potential equation (2) gives

$$\ln \Xi = \sum_{\ell=1}^{\infty} \frac{1}{\ell} \sum_{k=0}^{\infty} C_k (\ell \beta \hbar \omega)^{k-3} z^\ell = \sum_{k=0}^{\infty} C_k (\beta \hbar \omega)^{k-3} g_{4-k}(z).$$  \hspace{1cm} (53)

Then the number of particles is

$$N = \sum_{k=0}^{\infty} C_k (\beta \hbar \omega)^{k-3} g_{3-k}(z).$$  \hspace{1cm} (54)

The critical temperature is given by equation (54) at the limit $\mu \to 0$. However, at this limit, only the first two terms in the sum are convergent. In the usual treatment, all of the divergent terms are ignored [4, 9, 10, 23], and the result of the critical temperature only contains the first-order correction. In the following, we give the second-order correction to the critical temperature.

Taking advantage of the asymptotic expression of the Bose–Einstein integral equation (10), we have

$$N \approx \frac{C_0}{(\beta \hbar \omega)^3} \zeta(3) + \frac{C_1}{(\beta \hbar \omega)^2} \zeta(2) - \frac{C_2}{\beta \hbar \omega} \ln(-\beta \mu) + I_3,$$  \hspace{1cm} (55)

where we introduce

$$I_3 = \sum_{k=3}^{\infty} C_k (\beta \hbar \omega)^{k-3} \Gamma(k - 2) \frac{1}{(-\beta \mu)^{k-2}}.$$  \hspace{1cm} (56)

After introducing the integral form of the gamma function with the regularization parameter $s \to 0$, equation (13), we have
\[ I_3 = \frac{1}{\beta \mu} \int_0^\infty dx x^s e^{-x} \sum_{k=3}^\infty C_k \left( \frac{\beta \hbar \omega}{-\beta \mu} x \right)^{k-3} \]

\[ = \frac{1}{\beta \mu} \int_0^\infty dx x^s e^{-x} K \left( \frac{\hbar^2 x}{2m - \mu} \right) \]

\[ - \frac{C_0 \Gamma (s - 2)}{\beta \hbar \omega} \left( \frac{\mu}{\hbar \omega} \right)^2 \frac{C_1 \Gamma (s - 1) - \mu}{\beta \hbar \omega} - \frac{C_2 \Gamma (s)}{\beta \hbar \omega}, \]  

(57)

where we use the heat kernel equation (51) to obtain the divergent sum. The second and third terms in equation (57) contain positive powers of \( \mu \), so they vanish when \( \mu \to 0 \). The first term can be changed to a spectrum zeta function, i.e. a sum of the powers of the spectrum, by equation (16). Therefore, when \( \mu \to 0 \), we have

\[ I_3 = \Gamma (1 + s) \frac{(-\mu)^s}{\beta} \sum_{i=1}^\infty \frac{1}{E_i^{1+s}} - \frac{C_2}{\beta \hbar \omega} \Gamma (s). \]  

(58)

The sum of the excited-state spectrum can be obtained exactly as

\[ \sum_{i=1}^\infty \frac{1}{E_i^{1+s}} = \frac{1}{2 (\hbar \omega)^{1+s}} [\zeta (s - 1) + 3 \zeta (s) + 2 \zeta (s + 1)]. \]

(59)

When \( s \to 0 \), equation (58) becomes

\[ I_3 = \frac{1}{\beta \hbar \omega} \left( - \ln \frac{\hbar \omega}{-\mu} - \frac{19}{24} + \gamma_E \right), \]

(60)

where the coefficient equations (52) are used. In this result, the linearly divergent terms of \( s \) are canceled. Substituting equations (60) and (52) into equation (55) gives

\[ N = \frac{1}{(\beta \hbar \omega)^3} \zeta (3) + \frac{3}{2 (\beta \hbar \omega)^2} \zeta (2) + \frac{1}{\beta \hbar \omega} \left[ - \ln (\beta \hbar \omega) - \frac{19}{24} + \gamma_E \right]. \]

(61)

Just like the general case discussed in section 2, the logarithmically divergent terms of \( \mu \) are also canceled. This is a fully analytical result of the critical temperature. Since \( \beta \hbar \omega \ll 1 \) at the transition point, the last two terms correspond to the first- and second-order corrections. Then the critical temperature is approximately

\[ T_c \approx \frac{N^{1/3}}{\zeta^{1/3} (3)} \frac{\hbar \omega}{k_B} \left\{ 1 - \frac{\zeta (2)}{2 \zeta^{2/3} (3)} \frac{1}{N^{1/3}} + \frac{1}{9 \zeta^{1/3} (3)} \left[ - \ln \frac{N}{\zeta (3)} + \frac{\pi^4 + 38 - 48 \gamma_E}{16 \zeta (3)} \right] \frac{1}{N^{2/3}} \right\} \]

\[ = \frac{N^{1/3}}{\zeta^{1/3} (3)} \frac{\hbar \omega}{k_B} \left[ 1 - 0.7275 \frac{1}{N^{1/3}} - (0.1045 \ln N - 0.6045) \frac{1}{N^{2/3}} \right]. \]

(62)

The first-order correction in equation (62) is consistent with the results in [4, 9, 10, 23], and we also give the second-order correction.

4.2. Two-dimensional harmonic potentials

Even when the zero-point energy is suppressed, the spectrum of a particle in a two-dimensional isotropic harmonic potential is still given by equation (50), but the degeneracy is \( n + 1 \), so the heat kernel becomes

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\[ K(t) = \sum_{n=0}^{\infty} (n+1)e^{-nt} = \frac{e^{2t}}{(e^t - 1)^2} = \sum_{k=0}^{\infty} C_k t^{k-2}, \]  

where the expansion coefficients are

\[ C_0 = 1, C_1 = 1, C_2 = \frac{5}{12}, \ldots. \]

Then the grand potential equation (2) and the number of particles become

\[ \ln \Xi = \sum_{l=1}^{\infty} \frac{1}{l} \sum_{k=0}^{\infty} C_k \left( l \beta \hbar \omega \right)^{k-2} z^l = \sum_{k=0}^{\infty} C_k \left( \beta \hbar \omega \right)^{k-2} g_{3-k}(z), \]

\[ N = \sum_{k=0}^{\infty} C_k \left( \beta \hbar \omega \right)^{k-2} g_{2-k}(z). \]

At the limit \( \mu \to 0 \), by using the asymptotic form equation (10), we can rewrite the expression of the particle number as

\[ N \approx \frac{C_0}{(\beta \hbar \omega)^2 \zeta(2)} - \frac{C_1}{\beta \hbar \omega} \ln(-\beta \mu) + I_2, \]

where we introduce

\[ I_2 = \sum_{k=2}^{\infty} C_k \left( \beta \hbar \omega \right)^{k-2} \Gamma(k-1) \left( -\frac{1}{(-\beta \mu)^{k-1}}. \right) \]

Clearly different from that in the three-dimensional case, the second term in equation (66) is divergent. By using the integral form of the gamma function equation (13), we obtain

\[ I_2 = \frac{1}{(-\beta \mu)} \int_0^\infty dx x^s e^{-x} \sum_{k=2}^{\infty} C_k \left( \frac{x}{-\mu} \hbar \omega \right)^{k-2} K \left( \frac{x}{2m - \mu} \beta \hbar \omega \right) - \frac{C_0 \Gamma(s-1) - \mu}{\beta \hbar \omega} - \frac{C_1 \Gamma(s)}{\beta \hbar \omega}. \]

When \( \mu \to 0 \), the second term vanishes, and the first term becomes a sum of the spectrum,

\[ I_2 = \Gamma(1+s) \frac{(-\mu)^s}{\beta} \sum_{i=1}^{\infty} \frac{1}{E_i^{1+s}} - \frac{1}{\beta \hbar \omega} \Gamma(s), \]

where the coefficient equations (64) are substituted. The exact result of the sum of the excited-state spectrum is

\[ \sum_{i=1}^{\infty} \frac{1}{E_i^{1+s}} = \frac{1}{(\hbar \omega)^{1+s}} \left[ \zeta(s) + \zeta(1+s) \right]. \]
Then taking $s \to 0$ gives
\[ I_2 = \frac{1}{\beta \hbar \omega} \left( -\ln \frac{\hbar \omega}{-\mu} - \frac{1}{2} + \gamma_E \right). \tag{71} \]

The particle number equation (66) becomes
\[ N = \frac{1}{(\beta \hbar \omega)^2} \zeta(2) + \frac{1}{\beta \hbar \omega} \left( -\ln (\beta \hbar \omega) - \frac{1}{2} + \gamma_E \right). \tag{72} \]

Just as before, all of the divergent terms are canceled, so the critical temperature of BEC in the two-dimensional harmonic potential is
\[ T_c \approx \sqrt{\frac{N \hbar \omega}{\zeta(2) k_B}} \left[ 1 - \frac{1}{4\zeta^{1/2}(2)} \left( \ln \frac{N}{\zeta(2)} - 1 + 2\gamma_E \right) \frac{1}{N^{1/2}} \right] \]
\[ = \sqrt{\frac{N \hbar \omega}{\zeta(2) k_B}} \left[ 1 - (0.1949 \ln N - 0.0670) \frac{1}{N^{1/2}} \right]. \tag{73} \]

5. The second critical temperature of BEC

As is well known, when the BEC phase transition occurs, a large number of particles fall into the ground state and the ground state is macroscopically occupied. However, in some anisotropic systems, the behavior of the Bose gas may be more complicated. If there exists a set of quantum states which are very close to the ground state, a macroscopic number of particles may be distributed over the set of states. This phenomenon is called generalized BEC [26–28], which can be classified into three types [26, 27, 37]: type I (II) refers to the case where a finite (infinite) number of single-particle states are macroscopically occupied; type III refers to the case where the occupation of the set of states is a macroscopic fraction of the total particle number although none of these states is macroscopically occupied. Generalized BEC has been described in various geometries and external potentials, with and without interaction [38–40].

In [40], the authors discuss generalized BEC in some anisotropic systems in the thermodynamic limit, including slabs, squared beams, and ‘cigars’. They show that in these systems, ideal Bose gases undergo two kinds of phase transitions. Therefore, besides the conventional critical temperature $T_c$, there is a second critical temperature $T_m$ connected to the second phase transition. In this section, we take an anisotropic slab as an example to discuss the same problem without the assumption of the thermodynamic limit, and we give the correction of the boundary on the second critical temperature of BEC.

We consider a Bose gas in a highly anisotropic slab as described in section 3.1. As in [40], the side length of the slab takes the form $a = Le^{\omega L} \gg L$. The total particle number can be expressed as
where \( f(n_x, n_y, n_z) = (z^{-1}e^{\beta E(n_x, n_y, n_z)} - 1)^{-1} \) denotes the average particle number in the state \((n_x, n_y, n_z)\). In equation (74) we divide the total particle number into three parts: the ground-state particle number \( N_0(T)\), the number of particles in states with \( n_z = 1\) (not including the ground state) \( N_1(T)\), and the number of particles in states with \( n_z \geq 2\), \( N_2(T)\). The condition for the conventional BEC then is [40]

\[
N = N_2^{\text{max}}(T_c) .
\]  

(75)

Since at the transition point \( T_c \) the number of particles in states with \( n_z = 1 \) is negligible, \( N_2(T_c) \) can be replaced with the total number of excited-state particles. This means that the condition equation (75) is actually equivalent to the condition for the conventional BEC. The critical temperature \( T_c \), given in section 3.1, satisfies equation (41), or

\[
N = \frac{V}{\lambda^3} \zeta \left( \frac{3}{2} \right) + \frac{a^2}{2\lambda^2} \ln \left( \frac{\lambda^2}{16\pi L^2} \right) .
\]  

(76)

In contrast to the usual three-dimensional system, in the highly anisotropic slab, when \( T < T_c \), no single state is macroscopically occupied, but the entire band of states with \( n_z = 1 \) is macroscopically occupied, i.e. this is a type III generalized condensation. Only when the temperature is lower than the second critical temperature, \( T < T_m \), is the ground state macroscopically occupied. Then there is a coexistence of type III generalized condensation and the standard type I condensation in the ground state [40]. As a result, the second critical temperature \( T_m \) satisfies

\[
N = N_1^{\text{max}}(T_m) + N_2^{\text{max}}(T_m) .
\]  

(77)

In the following we discuss the influence of the boundary on the second critical temperature.

Since

\[
N_1(T) = \sum_{n_x, n_y=1}^{\infty} \frac{1}{z^{-1}e^{\beta E(n_x, n_y, 1)} - 1} - \frac{1}{z^{-1}e^{\beta E(1, 1, 1)} - 1},
\]  

(78)

when \( a \to \infty \), the sums of \( n_x, n_y \) can be converted to integrals, and we have

\[
N_1(T) = \frac{a^2}{\lambda^2} g_1(e^{-\beta\Delta}) - \frac{1}{e^{\beta\Delta} - 1},
\]  

(79)

where we introduce

\[
\Delta = \frac{\pi^2\hbar^2}{2mL^2} - \mu.
\]  

(80)

Near the second critical temperature, \( \beta\Delta \to 0 \); then
\[ N_1(T) \approx -\frac{a^2}{\lambda^2} \ln(\beta \Delta) - \frac{1}{\beta \Delta}. \]  

Since its maximum appears at \( \beta \Delta = \lambda_m^2/a^2 \), the condition for the phase transition equation (77) becomes

\[ N \approx \frac{a^2}{\lambda_m^2} \ln \left( \frac{a^2}{4\sqrt{\pi L} \lambda_m} \right) - \frac{a^2}{\lambda_m^2} + \zeta \left( \frac{3}{2} \right) \frac{V}{\lambda_m^3}. \]  

Substituting \( a = L e^{\alpha L} \) gives

\[ N = \frac{L^2 e^{2\alpha L}}{\lambda_m^2} \left[ 2\alpha L - 1 + \ln \left( \frac{L}{4\sqrt{\pi \lambda_m}} \right) \right] + \zeta \left( \frac{3}{2} \right) \frac{L^3 e^{2\alpha L}}{\lambda_m^3}. \]  

This is the equation that the second critical temperature \( T_m \) obeys. Using equation (76), we can obtain the relation between the two critical temperatures

\[ T_m^{3/2} + \frac{\xi}{L} T_m \left[ 2\alpha L - 1 + \frac{1}{2} \ln \left( \frac{L^2 mk}{32\pi^2 a^2} T_m \right) \right] = T_c^{3/2} - \frac{\xi}{2L} T_c \ln \left( \frac{L^2 mk}{8\hbar^2} T_c \right), \]  

where

\[ \xi = \frac{1}{\zeta (3/2)} \sqrt{ \frac{2\pi \hbar^2}{mk} }. \]  

It is easy to check that in the thermodynamic limit \( L \to \infty \), the relation (84) becomes

\[ T_m^{3/2} + 2\alpha \xi T_m = T_c^{3/2}, \]  

which is consistent with the result given in [40].

On the other hand, if we consider an isothermal process, the conditions for the phase transitions are described by the critical particle densities. According to equations (76) and (83), in an isothermal process, the two critical densities are

\[ n_c = \frac{\zeta (3/2)}{\lambda^3} + \frac{1}{L \lambda^2} \ln \left( \frac{\lambda}{4\sqrt{\pi L}} \right), \]
\[ n_m = \frac{\zeta (3/2)}{\lambda^3} + \frac{1}{L \lambda^2} \left[ 2\alpha L + \ln \left( \frac{L}{4\sqrt{\pi \lambda}} \right) - 1 \right]. \]  

Then we have

\[ n_m = n_c + \frac{2\alpha}{\lambda^2} + \frac{2}{L \lambda^2} \left( \ln \frac{L}{\lambda} - \frac{1}{2} \right). \]  

In the thermodynamic limit \( L \to \infty \), this relation goes back to the result in [40].

In the foregoing we have obtained the correction of the boundary to the second critical temperature of BEC in a slab geometry. A similar method can also be applied to systems with other anisotropic boundaries or external potentials.
6. Conclusion and discussion

We have discussed the critical temperature of the BEC of ideal gases in finite systems in a general framework based on the heat kernel expansion and zeta function regularization. Our method gives the analytical expression of the critical temperature related only to the heat kernel coefficients. We consider some specific examples and give the corresponding critical temperatures. Some of them have been obtained by other methods, but we provide a consistent treatment for different systems in this paper. Besides, taking advantage of the asymptotic spectrum, we separate the effect of the finite number of particles on the critical temperature from other factors, and the result agrees with the numerical calculation very well. For the Bose gas in isotropic harmonic traps, we obtain the second-order correction to the critical temperature for the three-dimensional case and the first-order correction for the two-dimensional case. In some highly anisotropic systems, besides the conventional BEC, generalized condensation may occur in a Bose system. We also give the correction of the boundary on the second critical temperature in an anisotropic slab. We hope that our work can help reveal the nature of the phase transition in finite systems.

In this paper, we only discuss the critical temperature of BEC. However, our method can also be applied to other aspects of the phase transition. For example, it can be used to analyze the properties of the thermodynamic functions, especially near the transition point. We leave these for future work.

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