Abstract. In two-dimensional traps, since the theoretical study of Bose–Einstein condensation will encounter the problem of divergence, the actual contribution of the divergent terms is often estimated in some indirect ways with the accuracy to the leading order. In this paper, by using an analytical continuation method to solve the divergence problem, we obtain the analytical expressions of critical temperature and condensate fraction for Bose gases in a 2D anisotropic box and harmonic trap, respectively. They are consistent with or better than previous studies. Then, we further consider the nonvanishing chemical potential, and obtain the expressions of chemical potential and more precise condensate fraction. These results agree with the numerical calculation well, especially for the case of harmonic traps. The comparison between the grand canonical and canonical ensembles shows that our calculation in the grand canonical ensemble is reliable.

Keywords: Bose Einstein condensation, quantum gases
1. Introduction

In recent years, Bose–Einstein condensation (BEC) in 2D systems attracts much research. First, the BEC of cold atoms in (quasi) 2D traps has been realized in experiments [1–3]. Then, more interestingly, the BEC of various bosonic quasiparticles in many-body systems has been widely investigated, such as excitons [4], magnons [5–7], cavity photons [8–10], and exciton-polaritons [11–13]. Many experiments of quasiparticles are realized in 2D traps.

In two dimensions, the realization of BEC is mainly in a box or harmonic trap. In the thermodynamic limit, these two cases have a remarkable difference: as the temperature descends, an ideal Bose gas in a 2D harmonic trap will undergo the BEC phase transition, but in 2D infinite space there is no phase transition. In finite systems, however, their difference becomes small since genuine phase transition cannot occur in either case. In both cases, at low enough temperature, a large fraction of particles will fall into the ground state, so the condensation can still occur. This kind of condensation phenomenon can be observed in experiments.

Unfortunately, there is an obstacle in the theoretical interpretation of the influence of trapping potentials or boundaries on the critical temperature of BEC for ideal Bose gases (We will still use the word 'critical temperature' in this paper though there is no genuine phase transition in a finite system). In the thermodynamic limit, the critical temperature is determined by the condition that the excited-state population \( N_e \) is equal to the total particle number \( N \) when the chemical potential \( \mu = 0 \). In a finite system, this condition can still be used as an approximate method. However, for trapped gases, the expression of \( N_e \) is usually divergent at \( \mu = 0 \). This problem is not too serious
for a 2D harmonic trap since the leading term is convergent. By neglecting all the other divergent terms, one can obtain the zero-order critical temperature, which is actually the result in the thermodynamic limit and is widely used in the literature [14–18]. In a 2D box, the problem is particularly serious since all terms of $N_e$ are divergent at $\mu = 0$. Then even the zero-order result cannot be obtained. In the literature, the critical temperature is determined by, for example, setting a given condensate fraction [19] or numerical calculation [20]. To obtain more precise results, the finite-size effect has been studied for many years, some approximate results of critical temperature and condensate fraction are also presented, often based on the analysis of the nonvanishing ground-state energy in a finite system and only including the leading correction [21–23]. A systematic method for studying the influence of potentials and boundaries is still lacking.

In this paper, we will use an analytical continuation method to deal with the divergence problem at $\mu = 0$, which is based on the heat kernel expansion and $\zeta$-function regularization [24]. First, we will show that the divergence can be removed by a general treatment, and the analytical expressions for critical temperature and condensate fraction for ideal Bose gases in a 2D anisotropic box or harmonic trap are presented, respectively. These results are consistent with or better than the previous studies. Then, more precisely, $\mu = 0$ does not exactly hold below the transition point in a finite system, but the divergence problem makes it difficult to solve the chemical potential. We will show that our method is applicable to this problem, and we will give the analytic expressions of the chemical potential and the more precise condensate fraction, respectively. These results agree with the numerical calculation well, especially for the harmonic traps. In addition, to check the influence of the fluctuation in the grand canonical ensemble, we compare the condensate fraction in the grand canonical and canonical ensembles. The comparison indicates that the difference between these two ensembles is very small for particle number $N \sim 10^3$.

The paper is organized as follows. In section 2, we discuss the BEC of an ideal Bose gas in a 2D rectangle box. The analytical expressions of the critical temperature, the condensate fraction, and the chemical potential are obtained. In section 3, we discuss the Bose gas in a 2D anisotropic harmonic trap. The first-order correction to the critical temperature, and the analytical expressions of condensate fraction and chemical potential are obtained. They agree with the numerical results very well. In section 4 we give a comparison between the grand canonical and canonical ensembles to show the influence of fluctuation in the grand canonical ensemble. The conclusion and some discussion are presented in section 5. A kind of the Epstein $\zeta$-function is used in our calculation, so we give its asymptotic expansion in appendix.

2. Two-dimensional rectangle box

The main tool used in this paper is the heat kernel expansion. In the grand canonical ensemble, the average particle number of an ideal Bose gas can be expanded as

$$\langle N \rangle = \sum_i \frac{1}{z^{-1} e^{\beta E_i} - 1} = \sum_{\ell=1}^{\infty} z^\ell \sum_i e^{-\ell \beta E_i} = \sum_{\ell=1}^{\infty} K \left( \frac{\ell \hbar^2}{2m \beta} \right) z^\ell,$$

(1)

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where \( z = e^{\beta \mu} \) is the fugacity, \( \beta = 1/(k_B T) \) with \( k_B \) denoting the Boltzmann constant, \( \{ E_i \} \) is the single-particle energy spectrum, which is proportional to the spectrum \( \{ \lambda_i \} \) of the Laplacian operator \( D = -\nabla^2 + (2m/\hbar^2) V(x) \), \( E_i = (\hbar^2/2m) \lambda_i \), and \( K(t) \) denotes the global heat kernel of the operator \( D \) \[25-27\]

\[
K(t) = \sum_{i=0}^{\infty} e^{-\lambda_i t}.
\]

(2)

For small \( t \), the heat kernel expansion of \( K(t) \) has the asymptotic form \[25-27\]

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

(3)

where \( d \) is the spatial dimension and \( B_k (k = 0, 1/2, 1, \cdots) \) are the heat kernel coefficients. Thus, equation (1) expresses the average particle number of the Bose gas as a series of global heat kernels.

In the thermodynamic limit, the critical temperature of BEC is determined by the condition that the excited-state population \( N_e \) equals the total particle number \( N \) at \( \mu = 0 \). In a finite system, although genuine phase transitions cannot occur, we can expect to obtain the critical temperature by the same condition as an approximation.

The excited-state population is easy to find from equation (1) by excluding the ground-state contribution. Furthermore, the transition occurring at \( \mu = 0 \) means that the ground-state energy should be zero, so we need to shift the energy spectrum so that the ground-state energy vanishes. In other words, we will replace the heat kernel equation (2) by

\[
K'(t) = \sum_{i=1}^{\infty} e^{-(\lambda_i-\lambda_0)t},
\]

(4)

in which the ground-state contribution is excluded. Therefore, for the 2D case, the corresponding heat kernel coefficients change to

\[
B_0' = B_0, B_{1/2}' = B_{1/2}, B_1' = B_1 + \lambda_0 B_0 - 4\pi, \cdots.
\]

(5)

In the following, we will consider a Bose gas in a 2D rectangle box of length sides \( L_x \) and \( L_y \) with Dirichlet boundary conditions. The shifted spectrum is

\[
\lambda(n_x, n_y) = \pi^2 \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right) - \pi^2 \left( \frac{1}{L_x^2} + \frac{1}{L_y^2} \right) \cdot (n_x, n_y = 1, 2, 3, \cdots).
\]

(6)

According to equation (5) and the usual heat kernel coefficients [28], the heat kernel coefficients for \( K'(t) \) are

\[
B_0' = S = L_x L_y, B_{1/2}' = -\sqrt{\pi}(L_x + L_y), B_1' = \pi^2 \left( \frac{L_y}{L_x} + \frac{L_x}{L_y} \right) - 3\pi, \cdots.
\]

(7)
Replacing the $K(t)$ in equation (1) by $K'(t)$, we can obtain the excited-state population as

$$N_e = \sum_{\ell=1}^{\infty} K'(\ell \frac{\hbar^2}{2m} \beta) z^\ell = \sum_{k=0,\frac{1}{2},1,\ldots}^{\infty} \frac{B'_k}{(4\pi)^k} \lambda^{2k-2} g_{1-k}(z),$$

where

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

is the Bose–Einstein integral, and $\lambda = \sqrt{2\pi\beta\hbar/\sqrt{m}}$ is the mean thermal wavelength. In equation (8) we have replaced $\langle N_e \rangle$ by $N_e$ for simplicity.

In equation (8), the heat kernel coefficient $B'_k$ has a dimension of $[L^{2-2k}]$. If we denote the characteristic length scale of the system as $\bar{L}$, $B'_k$ will be roughly proportional to $\bar{L}^{2-2k}$, just as in equation (7). Therefore, equation (8) is in fact a series of $\lambda/\bar{L}$.

### 2.1. Critical temperature $T_c$

The critical temperature of BEC is determined by $N_e = N$ at $\mu = 0$. In equation (8), $N_e$ is expressed as a series of a small parameter $\lambda/\bar{L}$, so usually the higher-order terms are just small corrections. However, when $\mu \to 0$, since the asymptotic behavior of the Bose–Einstein integral is

$$g_\sigma(e^{\beta\mu}) \approx \begin{cases} \zeta(\sigma), & (\sigma \geq \frac{3}{2}) \\ -\ln(-\beta\mu), & (\sigma = 1) \\ \Gamma(1-\sigma) \frac{1}{(-\beta\mu)^{1-\sigma}}, & (\sigma \leq \frac{1}{2}) \end{cases} \quad (\mu \to 0)$$

where $\zeta(\sigma) = \sum_{n=1}^{\infty} n^{-\sigma}$ is the Riemann zeta function, every term in equation (8) is divergent, and the divergence becomes more severe in the higher orders. As a result, it will not work to truncate this series at any finite order. To overcome this divergence problem, we will use an analytical continuation method with the help of the heat kernel expansion and $\zeta$-function regularization [24], in which all the terms in the series are considered.

First, substituting the leading term in the asymptotic expansion of the Bose–Einstein integral equation (10) into equation (8) gives

$$n_e \lambda^2 \approx -\ln(-\beta\mu) + \sum_{k=\frac{1}{2},\frac{3}{2},1,\ldots}^{\infty} \Gamma(k) \frac{B'_k}{(4\pi)^k S} \lambda^{2k-1} \frac{1}{(-\beta\mu)^k},$$

where $n_e = N_e/S$ is the number density of excited-state particles. We hope to express the divergent sum in equation (11) by the heat kernel. For this purpose, we introduce a regularization parameter $s$ which will be set to 0 at the end of the calculation in the gamma function

$$\Gamma(\xi) = \int_0^\infty x^{\xi-1}e^{-s} \, dx. \quad (s \to 0).$$
Equation (11) becomes

\[ n_e \lambda^2 = - \ln (-\beta \mu) + \int_0^\infty dx x^{-1+s} e^{-x} \left[ \frac{1}{S} \sum_{k=0, \frac{1}{2}, 1, \ldots} B_k^2 \left( \frac{\hbar^2}{2 m (-\mu)} x \right)^k - 1 \right] \]

\[ = - \ln (-\beta \mu) + \frac{2 \pi \hbar^2}{mS (-\mu)} \int_0^\infty dx x^s e^{-x} K' \left( \frac{\hbar^2}{2 m (-\mu)} x \right) - \Gamma(s). \] (13)

In the last line we have replaced the divergent series by the heat kernel \( K'(t) \) according to the heat kernel expansion.

Then, by the definition of heat kernel equation (4), we can perform the integral in equation (13),

\[ n_e \lambda^2 = - \ln (-\beta \mu) + \frac{2 \pi \hbar^2}{mS} \Gamma (1 + s) (-\mu)^s \sum' \frac{1}{[E(n_x, n_y) - \mu]^{1+s}} - \Gamma(s), \]

(14)

where the prime on the sum \( \sum' \) denotes that the ground state is excluded. Since the transition occurs at \( \mu = 0 \), by neglecting the chemical potential \( \mu \) in the denominator, the sum in equation (14) becomes

\[ \sum' \frac{1}{[E(n_x, n_y)]^{1+s}} = \left( \frac{2mS}{\pi^2 \hbar^2} \right)^{1+s} \sum_{(n_x, n_y) \neq (1,1)} \frac{1}{[\chi^{-1} n_x^2 + \chi n_y^2 - (\chi + \chi^{-1})]^{1+s}} \]

\[ = \left( \frac{2mS}{\pi^2 \hbar^2} \right)^{1+s} \sum_{p=0}^\infty \frac{1}{p} \left[ (\chi + \chi^{-1})^p E_2 \left( 1 + s + p, \chi^{-1}, \chi \right) - (\chi + \chi^{-1})^{-1-s} \right], \] (15)

where we have introduced a shape factor \( \chi = L_z / L_y \), and \( \binom{n}{k} = \frac{n!}{k!(n-k)!} \) is the binomial coefficient,

\[ E_2 (\sigma; a_1, a_2) = \sum_{n_1, n_2 = 1}^\infty \frac{1}{(a_1 n_1^2 + a_2 n_2^2)^\sigma} \]

is the Epstein \( \zeta \)-function. By use of equation (A.5) in appendix, when \( s \to 0 \), equation (15) is divergent and its asymptotic form is

\[ \sum' \frac{1}{[E(n_x, n_y)]^{1+s}} \approx \left( \frac{2mS}{\pi^2 \hbar^2} \right)^{1+s} \pi \left( \frac{1}{s + \Omega_2} \right), \] (17)

where

\[ \Omega_2 = 3 \gamma + \psi \left( \frac{1}{2} \right) - \frac{\pi}{3} (\chi + \chi^{-1}) - \frac{4 \pi}{\pi} (\chi + \chi^{-1})^{-1} - \text{ln} [\chi \eta^4 (i \chi)] \]

\[ + \frac{4}{\pi} \sum_{p=1}^\infty \left[ (\chi + \chi^{-1})^p E_2 \left( 1 + p, \chi^{-1}, \chi \right) - (\chi + \chi^{-1})^{-1} \right] \] (18)

is a parameter only related to the shape factor \( \chi \), \( \gamma \approx 0.5772 \) is the Euler constant, \( \psi(z) = \Gamma'(z) / \Gamma(z) \) is the digamma function, and

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\[ \eta(\tau) = e^{\pi i \tau} \prod_{n=1}^{\infty} \left(1 - e^{2n\pi i \tau}\right) \]  

(19)

is the Dedekind \( \eta \)-function. Since for \( s \to 0 \),

\[ \Gamma(s - n) \approx \frac{(-1)^n}{n!} \left[ \frac{1}{s} + \psi(n + 1) \right], \quad (n = 0, 1, 2, \ldots) \]  

(20)

the divergent term of \( s \) from equation (17) and that from the term with \( \Gamma(s) \) are exactly canceled.

Finally, equation (14) becomes

\[ n_c \lambda^2 = \ln \frac{2mS}{\pi^2 \hbar^2 \beta} + \Omega_2 = \ln \frac{N}{n \lambda^2} + \Omega, \]  

(21)

where we have introduced

\[ \Omega = \ln \frac{4}{\pi} + \Omega_2 \]  

(22)

for simplicity. In equation (21), all of the divergent terms of \( \mu \) are also canceled, and the final result is fully analytical, so the critical temperature is

\[ T_c = \frac{2\pi \hbar^2}{mk_B} \frac{n}{W(N e^{\Omega})}. \]  

(23)

where \( W(z) \) is the Lambert \( W \) function, satisfying \( z = W(ze^z) \).

Equation (23) gives the influence of the particle number and the shape of box on the critical temperature. In figure 1 we plot the relation between critical temperature and \( \chi \) at fixed density of particles. It shows that the anisotropy lowers the critical temperature. In this and the following figures, the temperature is rescaled to \( T/T_b \), where

\[ T_b = T_c (N = 1000, \chi = 1) \approx 0.228 \frac{2\pi \hbar^2 n}{mk_B} \]  

(24)

is the critical temperature for \( N = 1000 \) in a square box.

There are many studies on the BEC in cavities, most of them concentrate on the 3D cases [29, 30]. For 2D boxes, in [21], the authors give a relation between the critical temperature and particle number, which is similar to equation (21) but with \( \Omega = 0 \). In [20], the authors discuss the property of an ideal Bose gas in a square box in both the grand canonical ensemble and canonical ensemble in details. Their research is based on numerical calculation, and obtain an expression of critical temperature by fitting the numerical solution. By taking \( \chi = 1 \) so that \( \Omega = -1.0468 \) in equation (23), our result will go back to the square box case. The relation between the critical temperature and particle number given by equation (23) and [20] and [21] are shown in figure 2. Our result agrees with the numerical calculation in [20] quite well.

2.2. Condensate fraction and chemical potential

In the above discussion, the chemical potential \( \mu \) is assumed to be zero at the transition point. It implies that \( \mu = 0 \) holds for \( T < T_c \) just like in the thermodynamic limit.
case. Under this assumption, the condensate fraction can be directly obtained from equation (21):

\[
\frac{N_0^{(0)}}{N} = 1 - \frac{1}{n\lambda^2} \left( \ln \frac{N}{n\lambda^2} + \Omega \right),
\]

which will be called the zero-order condensate fraction in this paper.

The chemical potential \( \mu \) cannot be exactly zero at \( T < T_c \) in a finite system, but because of the divergence problem, directly solving \( \mu \) is difficult, especially near the
transition point. When $T \ll T_c$, $\mu$ can be approximate to $-k_B T / N_0^{(0)}$, but this approximation is invalid for $T \sim T_c$ since $N_0^{(0)} = 0$ at the transition point.

The discussion in the above section provides a way to avoid the divergence, so we can solve $\mu$ by the similar way. Specifically, accurate to $\mu^1$, we will add three more terms in equation (14) to obtain the expression of total particle number: the contribution from the ground-state particles

$$N_0^{(1)} = \frac{1}{e^{-\beta \mu} - 1} \approx \frac{1}{-\beta \mu},$$

(26)

the next-to-leading term in the asymptotic expansion of the Bose–Einstein integral in the first term

$$g_1 (e^{\beta \mu}) \approx -\ln ( -\beta \mu ) + \frac{-\beta \mu}{2},$$

(27)

and the first-order contribution of $\mu$ in the sum of energy spectrum

$$\sum' \frac{1}{[E(n_x, n_y) - \mu]^{1+s}} \approx \sum' \left\{ \frac{1}{[E(n_x, n_y)]^{1+s}} - \frac{(1 + s) (-\mu)}{[E(n_x, n_y)]^{2+s}} \right\}. \quad (28)$$

In the right-hand side of this equation, the first sum has been given in equation (17); the second sum is analytical at $s = 0$, so we can directly set $s = 0$ in it. By introducing a parameter only related to $\chi$,

$$\Omega_3 = \sum_{p=0}^{\infty} (p + 1) \left( \chi + \chi^{-1} \right)^p \left[ E_2 (p + 2; \chi^{-1}, \chi) - (\chi + \chi^{-1})^{-p-2} \right],$$

(29)

we can express the asymptotic expansion of equation (28) at $s \to 0$ as

$$\sum' \frac{1}{[E(n_x, n_y) - \mu]^{1+s}} \approx \left( \frac{2mS}{\pi^2 \hbar^2} \right)^{1+s} \left[ \frac{\pi}{4} \frac{1}{s} + \frac{\pi}{4} \Omega_2 - \frac{2mS}{\pi^2 \hbar^2} \Omega_3 \right]. \quad (30)$$

Thus, equation (14) with the additional terms becomes

$$n \lambda^2 \approx \frac{n \lambda^2}{N} \frac{1}{-\beta \mu} - \left( \frac{16 \Omega_3 N}{\pi^2} \frac{N}{n \lambda^2} - \frac{1}{2} \right) (-\beta \mu) + \ln \frac{N}{n \lambda^2} + \Omega,$$

(31)

where the divergent terms of $s$ have also been canceled. The term $-1/2$ in the parentheses in the second term can be neglected, which means that the contribution from the second term of $g_1 (e^{\beta \mu})$ in equation (27) is much smaller than that from the second term in the right-hand side of equation (28). After neglecting this small term, we can solve the chemical potential as

$$\mu \approx \mu_c \left[ \sqrt{1 + \frac{\pi^2}{64 \Omega_3} (n \lambda^2)^2 \left( \frac{N_0^{(0)}}{N} \right)^2} - \frac{\pi}{8 \sqrt{\Omega_3} n \lambda^2 N_0^{(0)}} \right],$$

(32)

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where

\[ \mu_c = -\frac{\pi^2 \hbar^2}{2\sqrt{\Omega_0}mS} \]  

(33)

is the chemical potential at the transition point.

In figure 3 we plot the relation between the chemical potential and temperature given by equation (32) for different \( N \). The result for \( \mu \) in the literature is rare, and we include the numerical results in the figure for comparison.

The first-order condensate fraction \( N_{(1)}^0/N \) in equation (26) is straightforward from equation (32). In figure 4 we show the relation between the condensate fraction and temperature for different \( N \). We can find that the zero-order condensate fraction \( N_{(0)}^0/N \) vanishes at the transition point as expected.

3. Two-dimensional anisotropic harmonic trap

The harmonic trap is the most commonly used trap in BEC experiments and also in the theoretical research. In fact, the thermodynamic properties of Bose gases in 2D harmonic traps can be exactly obtained \([31, 32]\). On the other hand, due to the divergence problem at the transition point, the critical temperature of BEC in a 2D harmonic trap is often approximately regarded as the thermodynamic-limit value \([14–18]\). In the following we will remove the divergence, and give the analytical forms of the critical temperature, the condensate fraction, and the chemical potential.

Consider an ideal Bose gas trapped in an anisotropic harmonic potential
$V = \frac{1}{2}m(\omega_x^2x^2 + \omega_y^2y^2)$. \hfill (34)

The single-particle energy spectrum has the form

$$E(n_x, n_y) = \hbar\omega_0 \lambda(n_x, n_y),$$ \hfill (35)

where $\omega_0 = \sqrt{\omega_x\omega_y}$ and

$$\lambda(n_x, n_y) = \sqrt{\kappa}n_x + \frac{1}{\sqrt{\kappa}}n_y, \quad (n_x, n_y = 0, 1, 2, \cdots)$$ \hfill (36)

where we have introduced $\kappa = \omega_x/\omega_y$ for convenience, and the ground-state energy has been shifted to 0. Consequently, the exact solution and the asymptotic expansion of the global heat kernel are

$$K(t) = \sum' e^{-\lambda(n_x, n_y)t} = \frac{1}{\left(1 - e^{-\sqrt{\kappa}t}\right)\left(1 - e^{-t/\sqrt{\kappa}}\right)} - 1$$
$$= \sum_{k=0}^{\infty} C_k t^{k-2}, \quad (t \to 0)$$ \hfill (37)

where $\sum'$ still represents that the ground state is excluded in the sum, and the expansion coefficients are

$$C_0 = 1, C_1 = \frac{1}{2}\left(\sqrt{\kappa} + \frac{1}{\sqrt{\kappa}}\right), C_2 = \frac{1}{12}\left(\kappa + \frac{1}{\kappa}\right) - \frac{3}{4}, \cdots.$$ \hfill (38)
In such a trap, the excited-state population of an ideal Bose gas is
\[ N_e = \sum_{\ell=1}^{\infty} z^\ell K(\ell \beta \hbar \omega_0) = \sum_{k=0}^{\infty} C_k (\beta \hbar \omega_0)^{k-2} g_{2-k} (z). \]  
(39)

### 3.1. Critical temperature \( T_c \)

To determine the critical temperature, we need to know the value of equation (39) at \( \mu = 0 \). However, under this condition, except the first term of equation (39), all the other ones are divergent. This divergence can also be removed by the method used in last section.

First, substituting the leading term of the asymptotic expansion of the Bose–Einstein integral equation (10) into equation (39) and replacing the gamma function by equation (12), we have
\[ N_e \approx \frac{C_0}{(\beta \hbar \omega_0)^2} \zeta (2) - \frac{C_1}{\beta \hbar \omega_0} \ln (-\beta \mu) + I_2, \]  
(40)

where
\[ I_2 = \frac{1}{(-\beta \mu)} \int_0^{\infty} dx x^s e^{-x} K \left( \frac{\hbar \omega_0}{-\mu} x \right) = \frac{C_0 \Gamma (s-1)}{(\beta \hbar \omega_0)^2} (-\beta \mu) - \frac{C_1 \Gamma (s)}{\beta \hbar \omega_0}. \]  
(41)

The integral in the first term becomes a sum over the spectrum,
\[ \frac{1}{(-\beta \mu)} \int_0^{\infty} dx x^s e^{-x} K \left( \frac{\hbar \omega_0}{-\mu} x \right) = \frac{\Gamma (1+s)}{\beta (\hbar \omega_y)^{1+s}} \sum' \frac{1}{(\kappa n_x + n_y - \frac{\mu}{\hbar \omega_y})^{1+s}}. \]  
(42)

For simplicity, we assume that \( \kappa \) is an integer. For \( \mu = 0 \), the sum then becomes
\[ \sum' \frac{1}{(\kappa n_x + n_y)^{1+s}} = \sum_{n=1}^{\infty} \sum_{n_x=0}^{[n]} \frac{1}{n^{1+s}}, \]  
(43)

where \( n = \kappa n_x + n_y \), and \([x]\) denotes the greatest integer not exceeding \( x \). Thus,
\[ \sum' \frac{1}{(\kappa n_x + n_y)^{1+s}} = \sum_{n=1}^{\infty} \left( \frac{n}{\kappa} + 1 \right) \frac{1}{n^{1+s}} - \sum_{k=1}^{\infty} \frac{k}{\kappa} \sum_{p=0}^{\kappa-1} \frac{1}{(pk + k)^{1+s}} \]
\[ = \frac{1}{\kappa} \zeta (s) + \zeta (1+s) - \sum_{k=1}^{\infty} \frac{k}{\kappa^{2+s}} \zeta (1+s, \frac{k}{\kappa}), \]  
(44)

where
\[ \zeta (s, a) = \sum_{n=0}^{\infty} \frac{1}{(n+a)^s}, (a \neq 0, -1, -2, \cdots) \]  
(45)
is the Hurwitz $\zeta$-function. Equation (44) is divergent at $s \to 0$, but the divergent term is exactly canceled by another divergent term coming from $\Gamma(s)$ in the last term in equation (41). Asymptotically expanding equation (41) at $s \to 0$ and dropping the term proportional to $\mu$, we have
\begin{equation}
I_2 = \frac{1}{2\beta \hbar \omega_y} \left[ \left( 1 + \frac{1}{\kappa} \right) \ln \frac{-\mu}{\hbar \omega_y} - \Delta \right],
\end{equation}
where
\begin{equation}
\Delta = \frac{1}{2\kappa} - \frac{1}{2} \left( 1 - \frac{1}{\kappa} \right) \ln \kappa - \sum_{k=1}^{\kappa-1} \frac{k}{\kappa^2} \psi \left( \frac{k}{\kappa} \right) - \gamma
\end{equation}
is a parameter only related to $\kappa$. Then equation (40) becomes
\begin{equation}
N_e = \frac{\zeta(2)}{\kappa (\beta \hbar \omega_y)^2} + \frac{1}{2\beta \hbar \omega_y} \left[ \left( 1 + \frac{1}{\kappa} \right) \ln \left( \frac{1}{\beta \hbar \omega_y} \right) - 2\Delta \right].
\end{equation}
In this equation, both of the divergent terms of $s$ and $\mu$ are canceled, so the critical temperature can be obtained analytically by setting $N_e = N$. Compared with the thermodynamic-limit result, the second term in the right-hand side in equation (48) is an extra correction. When the correction is small, the critical temperature is approximately
\begin{equation}
T_c \approx T_0 \left\{ 1 - \frac{\sqrt{6\kappa}}{8\pi} \frac{1}{\sqrt{N}} \left[ \left( 1 + \frac{1}{\kappa} \right) \left( \ln N + \ln \frac{6\kappa}{\pi^2} \right) - 4\Delta \right] \right\},
\end{equation}
where
\begin{equation}
T_0 = \frac{\sqrt{6N} \hbar \omega_0}{\pi k_B}
\end{equation}
is the critical temperature in the thermodynamic limit. The leading term in the correction to the critical temperature is proportional to $\ln N/\sqrt{N}$, which is consistent with the leading term of the quantum correction given in [23].

In figure 5, we plot the critical temperatures equations (49) and (50) for different $\kappa$. It shows that our result is lower than the thermodynamic-limit value ($T_c < T_0$), and the anisotropy increases the difference between them. In this and the following figures, the temperature is rescaled to $T/ T_h$, where $T_h = T_c (N = 1000, \kappa = 1)$.

### 3.2. Condensate fraction and chemical potential

Under the assumption $\mu = 0$, the zero-order condensate fraction is easy to obtain from equation (48),
\begin{equation}
\frac{N_0^{(0)}}{N} = 1 - \left( \frac{T}{T_0} \right)^2 - \frac{\sqrt{6} (\kappa + 1)}{4\pi \sqrt{\kappa N}} \frac{T}{T_0} \left\{ \ln \left[ \frac{6\kappa}{\pi^2} \left( \frac{T}{T_0} \right)^2 N \right] - \frac{4\kappa}{\kappa + 1} \Delta \right\}.
\end{equation}
For the isotropic case, i.e. $\kappa = 1$, neglecting the higher-order contribution in the third term, the zero-order condensate fraction can be expressed as
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\[ \frac{N_0^{(0)}}{N} \approx 1 - \left( \frac{T}{T_0} \right)^2 - \frac{\sqrt{6}}{2\pi} \frac{T \ln N}{T_0 \sqrt{N}}. \] (52)

In [22], the author gives an approximate result of the condensate fraction in an isotropic harmonic trap, which has the similar form as equation (52) but the coefficient of the third term is twice as large as our result. The comparison with the numerical calculation confirms that equation (52) is much more precise (see figure 7).

In a finite system, the chemical potential \( \mu \) is not exactly zero below the transition point. To find the analysis form of \( \mu \), we need to add three terms in equation (40) to give an equation of \( N \): the ground-state particle, the next-to-leading term of the Bose–Einstein integral, and the first-order correction of \( \mu \) in equation (42). Thus equation (40) becomes:

\[
N \approx \frac{1}{-\beta \mu} + \frac{C_0}{(\beta \hbar \omega_0)^2} \left[ \zeta(2) - \beta \mu \ln \left( -\beta \mu \right) - 1 \right] - \frac{C_1}{\beta \hbar \omega_0} \ln \left( -\beta \mu \right) \\
+ \frac{\Gamma(1 + s)(-\mu)^s}{\beta (\hbar \omega_y)^{1+s}} \sum' \frac{1}{(\kappa n_x + n_y - \mu_{\omega_y})^{1+s}} - \frac{C_0 \Gamma(s - 1)}{(\beta \hbar \omega_0)^2} (-\beta \mu) - \frac{C_1 \Gamma(s)}{\beta \hbar \omega_0}. 
\] (53)

The sum of the spectrum is approximately

\[
\sum' \frac{1}{(\kappa n_x + n_y - \mu_{\omega_y})^{1+s}} \approx \sum' \left[ \frac{1}{(\kappa n_x + n_y)^{1+s}} - \frac{(1 + s)(-\mu)}{\hbar \omega_y (\kappa n_x + n_y)^{2+s}} \right]. \quad (54)
\]

The first term has been calculated in equation (44), and the second term is also divergent at \( s \to 0 \): \n\[
\frac{\Gamma(1 + s)(-\mu)^s}{\beta (\hbar \omega_y)^{1+s}} \sum' \frac{(1 + s)(-\mu)}{\hbar \omega_y (\kappa n_x + n_y)^{2+s}} = \frac{-\mu}{\kappa \beta (\hbar \omega_y)^2} \left( \frac{1}{s} + \ln \frac{-\mu}{\hbar \omega_y} - \gamma + \Delta_2 \right), \quad (55)
\]

Figure 5. The influence of anisotropy on the critical temperature in a 2D harmonic trap for \( N = 1000 \). The anisotropy increases the difference between \( T_c \) and \( T_0 \).
where
\[ \Delta_2 = \gamma + 1 + \frac{\pi^2}{6} \kappa - \sum_{k=1}^{\kappa-1} \frac{k}{\kappa^2} \zeta \left( 2, \frac{k}{\kappa} \right) \]  \hspace{1cm} (56)

is only related to \( \kappa \). However, the term with \( \Gamma(s-1) \) in equation (53) is proportional to \( \mu \) and should be included in this approximation. Easy to check that the divergent term coming from the gamma function and that in equation (55) are exactly canceled. Therefore all the divergent terms of \( s \) are canceled in equation (53):
\[ N = \frac{1}{-\beta \mu} + \frac{\zeta(2)}{\kappa (\beta \hbar \omega_y)^2} + \frac{1}{\beta \hbar \omega_y} \left[ \frac{1}{2} \left( 1 + \frac{1}{\kappa} \right) \ln \frac{1}{\beta \hbar \omega_y} - \Delta \right] - \frac{-\beta \mu}{\kappa (\beta \hbar \omega_y)^2} \left( \ln \frac{1}{\beta \hbar \omega_y} + \Delta_2 \right). \]  \hspace{1cm} (57)

By using equations (51) and (50), it can be rewritten as
\[ N_0^{(0)} = \frac{1}{-\beta \mu} - \frac{6N}{2\pi^2} \left( \frac{T}{T_0} \right)^2 \left\{ \ln \left[ \frac{6\kappa N}{\pi^2} \left( \frac{T}{T_0} \right)^2 \right] + 2\Delta_2 \right\} (-\beta \mu). \]  \hspace{1cm} (58)

Neglecting the higher-order terms, we solve the chemical potential as
\[ \mu \approx \mu_c \left[ \sqrt{1 + \frac{\pi^2}{12} \left( \frac{T}{T_0} \right)^2 \frac{N_0^{(0)2}}{N \ln N} - \frac{\pi}{2\sqrt{3}} \frac{T_0}{T} \frac{N_0^{(0)}}{\sqrt{N \ln N}} } \right], \]  \hspace{1cm} (59)

where
\[ \mu_c = -\sqrt{\frac{2}{\ln N}} \hbar \omega_0 \]  \hspace{1cm} (60)

is the chemical potential at the transition point.

In figure 6 we plot the relation between the chemical potential and temperature for different \( N \). For \( T < T_c \), equation (59) agrees with the numerical solution quite good.

From equation (59), the first-order condensate fraction \( N_0^{(1)}/N \) is straightforward according to equation (26). In figure 7 we plot the relation between the condensate fraction and temperature for different \( N \). At the critical temperature, the zero-order condensate fraction vanishes, but the first-order one matches the numerical solution very well.

4. Comparison with the canonical ensemble

In the above sections, our discussion on BEC is in the grand canonical ensemble. However, in a finite system, the fluctuation of particle number in the grand canonical ensemble may be non-negligible. For investigating the influence of fluctuation, we will consider the behavior of Bose gases in the canonical ensemble and compare the result with the grand canonical ensemble.
There are many studies on the similarities and differences between different ensembles for finite systems [14, 20, 33, 34]. In this section, we will take the 2D harmonic trap as an example to show the difference between these two ensembles.

In the canonical ensemble, the partition function of a $N$-particle system is

$$Q(N) = \sum_k e^{-\beta E_k^{(S)}},$$

(Figure 6. The relation between chemical potential and temperature for different $N$ in a 2D isotropic harmonic trap ($\kappa = 1$). Our result matches the numerical solution very well. The three sets of lines denote $N = 300, 1000, 3000$ from left to right.

Figure 7. The relation between condensate fraction and temperature for different $N$ in a 2D isotropic harmonic trap ($\kappa = 1$). The result of [22], the numerical solution, the zero- and first-order approximations are plotted for $N = 300, 1000, 3000$ from left to right.)
where $E_k^{(S)}$ is the total energy of the $k$th system in the ensemble. However, the constraint of fixed particle number makes the exact analytical form of partition function for a quantum system hard to obtain, even for ideal gases. One method is to express the partition function by a complex integral of the grand partition function as

$$Q(N) = \frac{1}{2\pi i} \oint z^{-N-1}\Xi(z)dz,$$

(62)

where the integral path is a loop surrounding the original point. However, although this integral can be approximately evaluated by the saddle point method for large $N$, the exact integral can hardly be performed.

To give a direct comparison between different ensembles, we need the exact partition function. For not very large $N$, this can be achieved by use of the recursion relation [20, 33]

$$Q(N) = \frac{1}{N} \sum_{k=1}^{N} Q_1(k)Q(N-k), \quad (Q(0) = 1)$$

(63)

where

$$Q_1(k) = \sum_i e^{-k\beta E_i}$$

(64)

is the partition function for a single particle at the temperature $T/k$.

We will take the condensate fraction as an example to compare with that in the grand canonical ensemble. The average particle number in a state with energy $E_i$ in the canonical ensemble can be expressed as [20, 33]
\[ \bar{N}_i = \frac{1}{Q(N)} \sum_{k=1}^{N} e^{-k\beta E_i} Q(N-k). \]  

(65)

Combined with equation (63), it will give the particle number in the ground state and the condensate fraction.

In figure 8 we plot the numerical solutions of condensate fraction in the grand canonical and canonical ensembles for different \( N \) in a 2D harmonic trap. It is clear that for \( N \sim 10^3 \), the difference between these two ensembles is very small.

5. Conclusion and discussion

In the above, by using an analytical continuation method to solve the divergence problem in BEC, we discuss the low-temperature behavior of ideal Bose gases in the 2D anisotropic box and harmonic trap, respectively. We show that the influence of boundaries and external potentials can be dealt with by a general treatment. We obtain the critical temperature, the condensate fraction and the chemical potential for Bose gases in these two kinds of traps, respectively. The results are consistent with or better than the corresponding studies in the literature, and they agree with the numerical calculation well. To check the influence of fluctuation in the grand canonical ensemble, we compare the condensate fraction in the grand canonical and canonical ensembles. The result shows that for about \( N \sim 10^3 \), the difference between these two ensembles is negligible.

Although some previous studies also discussed the corrections to critical temperature and condensate fraction in finite systems, our method is not an order-of-magnitude estimate, so we can obtain more precise results, including not only the leading correction. Besides, our method provides a general treatment to the problem of BEC in finite systems. As long as the heat kernel expansion is known, the critical temperature and the thermodynamic quantities of the Bose gas can be calculated.

The grand potential of a finite system also contains divergent terms at \( \mu \to 0 \), and this problem can also be solved by similar treatment. The analytical expressions of the grand potential and other thermodynamic quantities below the transition point can be obtained as well. However, the divergence problem is often not serious in the grand potential. For the two cases considered in this paper, the divergence appears from the third term of the grand potential. Therefore, our method will give the corrections to the third terms. Such corrections are usually negligible, so their expressions are not presented in this paper.

The advantage of our method is to remove the divergence at the transition point, so the magnitude of the correction tightly depends on the specific nature of the systems. For example, for the critical temperature, it gives the second-order correction in the case of 3D harmonic traps, which is usually negligible [24]. In a 2D harmonic trap, the correction is first-order and is expected to be observed in experiments. In a 2D box, since no phase transition exists in the thermodynamic limit, the correction is zero-order and its influence is significant.
Recently, many experimental studies on BEC are performed in 2D traps, especially the BEC of quasiparticles, such as excitons in graphene and surface exciton-polaritons. We hope that more precise experiments at this field will test our results.

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Appendix. Asymptotic expansion of the Epstein $\zeta$-function $E_2(\sigma; a_1, a_2)$

According to [35], the Epstein $\zeta$-function

$$E_2(\sigma; a_1, a_2) = -\frac{1}{2} a_2^{-\sigma} \zeta(2\sigma) + \frac{1}{2} a_2^{-\sigma} \sqrt{\frac{\pi a_2}{a_1}} \frac{\Gamma(\sigma - 1/2)}{\Gamma(\sigma)} \zeta(2\sigma - 1)$$

$$+ \frac{2\pi - \frac{3}{4} a_1^{-\sigma - 1} a_2^{-\frac{3}{4}} \Gamma(\sigma)}{\Gamma(\sigma)} \sum_{n_1, n_2=1}^{\infty} n_1^{-\frac{1}{2}} n_2^{-\frac{3}{4}} K_{\sigma - 1/2} \left(2\pi \sqrt{\frac{a_2}{a_1}} n_1 n_2\right) \tag{A.1}$$

has a singularity $\sigma = 1$, so we need the asymptotic expansion of Epstein $\zeta$-function around $\sigma = 1$.

Around $\sigma = 1$, only the second term in equation (A.1) is divergent, which is

$$\frac{1}{2} a_2^{-\sigma} \sqrt{\frac{\pi a_2}{a_1}} \frac{\Gamma(\sigma - 1/2)}{\Gamma(\sigma)} \zeta(2\sigma - 1)$$

$$\approx \frac{\pi}{4} a_1 a_2 \left[ \frac{1}{\sigma - 1} + 3\gamma + \psi \left(\frac{1}{2}\right) - \ln a_2 \right]. \tag{A.2}$$

The first and third terms in equation (A.1) is convergent, so substituting $\sigma = 1$ into them gives

$$-\frac{1}{2} a_2^{-1} \zeta(2) = -\frac{\pi^2}{12a_2} \tag{A.3}$$

and

$$2\pi a_1^{-\frac{3}{4}} a_2^{-\frac{1}{4}} \sum_{n_1, n_2=1}^{\infty} n_1^{-\frac{1}{2}} n_2^{-\frac{3}{4}} K_{1/2} \left(2\pi \sqrt{\frac{a_2}{a_1}} n_1 n_2\right)$$

$$= 2\pi a_1^{-\frac{3}{4}} a_2^{-\frac{1}{4}} \left(\frac{a_1}{a_2}\right)^{1/4} \sum_{n_1, n_2=1}^{\infty} \frac{1}{n_2} e^{-2\pi \sqrt{\frac{a_2}{a_1}} n_1 n_2}$$

$$= -\frac{\pi^2}{12a_1} - \frac{\pi}{\sqrt{a_1 a_2}} \ln \left(i \sqrt{\frac{a_2}{a_1}} \right). \tag{A.4}$$

Therefore, around $\sigma = 1$, we have
\begin{equation}
E_2(\sigma; a_1, a_2) \approx \frac{\pi}{4\sqrt{a_1a_2}} \frac{1}{\sigma - 1} - \frac{\pi^2}{12} \left( \frac{1}{a_1} + \frac{1}{a_2} \right) + \frac{\pi}{4\sqrt{a_1a_2}} \left[ 3\gamma + \psi \left( \frac{1}{2} \right) - \ln \left( a_2 \eta^4 \left( i \sqrt{\frac{a_2}{a_1}} \right) \right) \right].
\end{equation}

References

[1] Görlitz A et al 2001 Phys. Rev. Lett. 87 130402
[2] Krüger P, Hadzibabic Z and Dalibard J 2007 Phys. Rev. Lett. 99 040402
[3] Chomaz L, Corman L, Bienaimé T, Desbuquois R, Weitenberg C, Nascimbène S, Beugnon J and Dalibard J 2015 Nat. Commun. 6 6162
[4] Eisenstein J P and MacDonald A H 2004 Nature 432 691
[5] Nikuni T, Oshikawa M, Oosawa A and Tanaka H 2000 Phys. Rev. Lett. 84 5868
[6] Demokritov S O, Demidov V E, Dzyapko O, Melkov G A, Serga A A, Hillebrands B and Slavin A N 2006 Nature 443 430
[7] Giamarchi T, Ruegg C and Tchernyshyov O 2008 Nat. Phys. 4 198
[8] Klaers J, Schmitt J, Vewinger F and Weitz M 2010 Nature 468 545
[9] Klaers J, Vewinger F and Weitz M 2010 Nat. Phys. 6 512
[10] Schmitt J, Damm T, Dung D, Vewinger F, Klaers J and Weitz M 2014 Phys. Rev. Lett. 112 030401
[11] Kasprzak J et al 2006 Nature 443 409
[12] Balili R, Hartwell V, Smoke D, Pfeiffer L and West K 2007 Science 316 1007
[13] Sun Y, Wen P, Yoon Y, Liu G, Steger M, Pfeiffer L N, West K, Smoke D W and Nelson K A 2017 Phys. Rev. Lett. 118 016602
[14] Haugset T, Haugerud H and Andersen J O 1997 Phys. Rev. A 55 2922
[15] Bagno V, Pritchard D E and Kleppner D 1987 Phys. Rev. A 35 4354
[16] Dalfövo F, Giorgini S, Pitaevskii L P and Stringari S 1999 Rev. Mod. Phys. 71 463
[17] Berman O L, Lozovik Y E and Smoke D W 2008 Phys. Rev. B 77 155317
[18] Berman O L, Kezerashvili R Y and Lozovik Y E 2009 Phys. Rev. B 80 115302
[19] Jiang J and John S 2014 Phys. Rev. X 4 031025
[20] Li H, Guo Q, Jiang J and Johnston D C 2015 Phys. Rev. E 92 062109
[21] Ketterle W and van Druten N J 1996 Phys. Rev. A 54 656
[22] Mullin W J 1997 J. Low Temp. Phys. 106 615
[23] Yukalov V I 2016 Laser Phys. 26 062001
[24] Xie M 2018 J. Stat. Mech. 053109
[25] Vassilevich D V 2003 Phys. Rep. 388 279
[26] Gilkey P B 2004 Asymptotic Formulae in Spectral Geometry (Boca Raton, FL: CRC Press)
[27] Dai W-S and Xie M 2009 Phys. Rev. A 76 063604
[28] Grossmann S and Holthaus M 1995 Z. Phys. B 97 319
[29] Kirsten K and Toms D J 1999 Phys. Rev. E 59 158
[30] Mullin W J and Fernández J P 2003 Am. J. Phys. 71 661
[31] Glaum K, Kleinert H and Pelster A 2007 Phys. Rev. A 76 063604
[32] Elizalde E and Romeo A 1989 Rev. Math. Phys. 1 113

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