Thermodynamic properties of a finite Bose gas in a harmonic trap*

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We have investigated the thermodynamic behaviour of ideal Bose gases with an arbitrary number of particles confined in a harmonic potential. By taking into account the conservation of the total number N of particles and using a saddle-point approximation, we derive analytically the simple explicit expression of mean occupation number in any state of the finite system. The temperature dependence of the chemical potential, specific heat, and condensate fraction for the trapped finite-size Bose system is obtained numerically. We compare our results with the usual treatment which is based on the grand canonical ensemble. It is shown that there exists a considerable difference between them at sufficiently low temperatures, especially for the relative small numbers of Bose atoms. The finite-size scaling at the transition temperature for the harmonically trapped systems is also discussed. We find that the scaled condensate fractions for various system sizes and temperatures collapse onto a single scaled form.

Keywords: trapped finite bosons, simple explicit distribution law, thermodynamics, finite-size scaling

PACC: 0530C, 6740K

1. Introduction

The observation of a remarkable series of experiments on Bose–Einstein condensation (BEC)[1−5] has encouraged a number of theoretical investigations for this state of matter. The BEC of free ideal Bose gas in the thermodynamic limit, as one of the traditional text book examples,[6] is usually described in the grand canonical ensemble. However, in the existing BEC experiments the trapped systems are always performed with a finite number of particles, which implies that the canonical ensemble is more appropriate. The research of BEC has been shifted from the traditional textbook examples of the homogeneous free gas in the thermodynamic limit to the systems containing a finite number of particles trapped in external potentials.[7−46]

A challenging work is to find a solution to the fundamental problem: how to describe the quantum 'phase transitions' for small systems far away from the thermodynamic limit? The small systems do not exhibit phase transitions.[33] The transition point is usually defined as a critical temperature at the maximum value of specific heat which shows a more or less smooth hump extending over some finite temperature range for the fixed and finite numbers of particles. To describe the BEC of a finite number of bosons trapped in three-dimensional (3D) potential, there have been mainly three kinds of approaches in recent decades. One of them is based on the grand canonical statistics. The effect of finite numbers of bosons on the BEC of ideal Bose gases in the 3D harmonic trap has been addressed a number of publications.[8−13,15,16] The second approach is based on the canonical statistics which have taken an increasing interest in recent years.[14,19−37,45] The third one is based on the master equation approach.[38,39,41,42] It yields analytical expressions for the distribution function of the number of condensed atoms and for the canonical partition function.

Even beyond the grand canonical statistics, the approach is valid for the total number of particles $N \gg 1$.[7−13,15] Although the theory is exact and self-consistent for an arbitrary number of particles in the canonical ensemble,[19−32,35−37,45] the calculations are heavily complicated with an increasing particle number of systems. For example, the computations of the canonical partition functions are always formidable tasks even for systems with a small number of particles. The master equation gives the most accurate and physically transparent picture of the BEC fluctuations. From the practical point of view, it is however limited to numerical results for moderate particle

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numbers.

Let us return to the early study on the quantum statistics. There were several ways to generalize the ordinary statistics in the textbooks. One is the parastatistics,[47] in which a wavefunction in a state vector can be antisymmetric with respect to at most p particles, though the maximum occupation number is infinite. The other one is the intermediate statistics proposed by Gentile.[48,49] in which a 1-particle state can be occupied by up to finite M_v particles for the v'th energy level. One way of the generalization is the Haldane statistics,[50] a most known fractional statistics. To the best of our knowledge, only the Haldane statistics has physical meaning in nature. In order to provide simple approximately analytical results and physical insights into the very complicated problem, we shall develop the Gentile approach for the Bose system with a particular form as a physical case: the maximum number of particles in every energy level is just the total number N of the system under consideration.

Under the usual saddle-point approximation, we derive the general expression for mean occupation number at any trapping state. The calculations of the thermodynamical quantities are very simple due to the analytical expressions for the mean occupation numbers. Therefore, the calculation in our work is very easy and simple. Since the system contains an arbitrary particle number, we use the finite-size scaling theory to explore the relation between the scaled condensate fraction and the scaled temperature in the case of an ideal nonuniform gas. This is also of interest since the finite-size scaling analysis was discussed only for interacting homogeneous Bose gases,[51−53] while the finite-size effects on the transition temperature and the finite-size scaling for the ideal trapped Bose gases are not reported. Through the finite-size scaling analysis we show that the condensate fractions for the various system sizes collapse to a single scaled form which has been proposed theoretically.[51−53]

The paper is organized as follows. In Section 2, by use of a saddle-point approximation, we derive the simple explicit expression of average occupation number in any state for the finite Bose system. In Section 3 we obtain the expressions for the specific heat, the condensate occupation number, and determine their temperature dependence. The numerical analysis is presented in Section 4, where the calculated results are compared with those in the grand canonical ensemble. The finite-size scaling of condensate fraction is also discussed. The main conclusions are given in Section 5.

2. Mean occupation number and distribution law

In ordinary Bose statistics, the number of particles n_v occupying the vth energy level can be any integer value $n_v = 0,\ 1,\ 2, \ldots$, and the total number of particles satisfies the condition $N = \sum_{v=0}^{\infty} n_v$ for a fixed N. The canonical partition function is defined as

$$Z_N = \sum_{\{n_v\}}^{M_v} \prod_v \mathrm{e}^{-\beta n_v \epsilon_v} \delta_{N,\ \sum_j n_j}, \quad (v, j = 0, 1, 2, \ldots) \tag{1}$$

with ϵ_v being the energy levels of N ideal particles and $\beta = 1/k_{\mathrm{B}}T$. A set of distributions is $\{n_v\}$ with various possibilities and it satisfies the Kronecker-delta relation which ensures that the system contains exactly N particles with $\max\{n_v\} \equiv M_v$ and $M_v \geq N$ for the bosons.[54] By use of the definition of delta function[54]

$$\delta_{N,\ \sum_j n_j} = \frac{1}{2\pi i} \int_{-\pi\,\mathrm{i}}^{\pi\,\mathrm{i}} \exp\left[-\Big(N - \sum_j n_j\Big)\lambda\right] \mathrm{d}\lambda, \tag{2}$$

the sum over states translates into the integral and Eq. (1) becomes

$$Z_N = \frac{1}{2\pi\,\mathrm{i}} \int_{-\pi\,\mathrm{i}}^{\pi\,\mathrm{i}} \mathrm{e}^{-N\lambda} \sum_{n_v}^{N} \prod_v \mathrm{e}^{(\lambda - \beta\epsilon_v) n_v} \mathrm{d}\lambda, \tag{3}$$

where $\sum_{n_v}^{N} = \sum_{n_0, n_1, \ldots, n_v, \ldots}^{N}$ under the condition $\sum_{v=0}^{\infty} n_v = N$ for n_v being the particle numbers in the vth state. It is noteworthy that when N approaches ∞ the restriction on the summation over n_v in Eq. (3) is in fact removed, which means that the result would be nothing more than the grand canonical partition function. In Eq. (3) we have replaced M_v in Eq. (1) by N because the system contains exactly N particles. Letting $\mathrm{e}^{\lambda - \beta\epsilon_v} \equiv x_v$, we thus have

$$\begin{aligned} \sum_{n_v}^{N} \prod_v x_v^{n_v} &= \sum_{n_0, n_1, \ldots, n_v, \ldots}^{N} x_0^{n_0} x_1^{n_1} \ldots x_v^{n_v} \ldots \\ &= \sum_{\ldots, n_v, \ldots}^{M_v} \Big(\sum_{n_0=0}^{M_0} x_0^{n_0} \Big) \Big(\sum_{n_1=0}^{M_1} x_1^{n_1} \Big) \ldots x_v^{n_v} \ldots \\ &= \prod_v \sum_{n_v=0}^{M_v} x_v^{n_v} \end{aligned} \tag{4}$$

with $M_v \leq N$ due to the constrained condition $\sum_{v=0}^{\infty} n_v = N$. For $N \to \infty$, Eq. (4) is satisfied exactly. While for finite N, if $\sum_{v=0}^{J} n_v = N$, then

$n_k = 0$ and $x_k^{n_k} = 1$ for $k \geq J+1$. The last equation in Eq. (4) is satisfied approximatively only if the energy level is not large enough. This approximation is valid for the condensate and low-level excitations in the trapped potential. Although we do not know the exact value of M_v in the finite Bose systems, we shall choose all $M_v = N$ through considering both the conditions $M_v \geq N$ in Eq. (1) and $M_v \leq N$ in Eq. (4). This follows from the fact that, for a system of finite number N of particles, the maximum occupation number in every level does not exceed the total particle number N.

Equation (3) can therefore be written as

$$Z_N = \frac{1}{2\pi\,\mathrm{i}} \int_{-\pi\,\mathrm{i}}^{\pi\,\mathrm{i}} \mathrm{e}^{-N\lambda} \prod_v \sum_{n_v}^{N} \mathrm{e}^{(\lambda-\beta\epsilon_v)n_v} \mathrm{d}\lambda, \qquad (5)$$

and the values of the numbers n_v must satisfy the condition $\sum_{v=0}^{\infty} n_v = N$. In Eq. (5) we have replaced '$\sum_{n_v}\prod_v$' by '$\prod_v \sum_{n_v}$' of Eq. (3), and therefore Eq. (5) can be applied directly to calculation. Carrying out the summation in Eq. (5), the canonical partition becomes

$$Z_N = \frac{1}{2\pi\,\mathrm{i}} \int_{-\pi\,\mathrm{i}}^{\pi\,\mathrm{i}} \mathrm{e}^{-N\lambda} \prod_v \frac{1-\mathrm{e}^{(N+1)(\lambda-\beta\epsilon_v)}}{1-\mathrm{e}^{\lambda-\beta\epsilon_v}} \mathrm{d}\lambda. \qquad (6)$$

Clearly, in the standard grand canonical ensemble and thermodynamic limit ($N \to \infty$), n_v can be any integer value, i.e., n_v from 0 to ∞, and the summation

$$\sum_{n_v=0}^{\infty} \mathrm{e}^{(\lambda-\beta\epsilon_v)n_v} = \frac{1}{1-\mathrm{e}^{\lambda-\beta\epsilon_v}}$$

is in the usual form. But now it is hard to evaluate Z_N explicitly. To proceed, we define $z = \mathrm{e}^{\lambda}$ and $z^{-N-1}\prod_v [1-z^{(N+1)}\mathrm{e}^{-(N+1)\beta\epsilon_v}]/(1-z\mathrm{e}^{-\beta\epsilon_v}) = \mathrm{e}^{F(z)}$, then Eq. (6) becomes

$$Z_N = \frac{1}{2\pi\,\mathrm{i}} \oint \mathrm{e}^{F(z)} \mathrm{d}z, \qquad (7)$$

where the contour of integration is a closed path in the complex z plane about $z = 0$. The saddle-point z_0 is determined by[55] $\frac{\partial F(z)}{\partial z}\,|_{z=z_0} = 0$. From this we obtain

$$N = \sum_{v=0}^{\infty} \left[\frac{1}{z_0^{-1}\mathrm{e}^{\beta\epsilon_v} - 1} - \frac{N+1}{z_0^{-(N+1)}\mathrm{e}^{(N+1)\beta\epsilon_v} - 1} \right], \qquad (8)$$

where the term of one extra particle on the left hand side has been neglected. Note that the saddle point z_0 can be regarded as the fugacity of N ideal bosons, and Eq. (8) is exactly the equation to determine this fugacity $z_0 = \mathrm{e}^{\beta\mu}$. From Eq. (8), in terms of the chemical potential μ the mean occupation numbers in the vth level now reads

$$n_v = \frac{1}{\mathrm{e}^{\beta(\epsilon_v-\mu)} - 1} - \frac{N+1}{\mathrm{e}^{(N+1)\beta(\epsilon_v-\mu)} - 1}. \qquad (9)$$

The expression for the mean occupation numbers in Eq. (9) is identical with the particular form of distribution law for the occupation numbers proposed by Gentile[48] on somewhat different grounds. In other words, the saddle point method is one of the methods to find the most probable distribution. If the particle number N is infinite, we should replace the finite sums in Eq. (5) by the infinite series. Then Eq. (9) should turn out to be the mean occupation numbers in the standard grand canonical ensemble, i.e., $n_v^0 = 1/(\mathrm{e}^{\beta(\epsilon_v-\mu)} - 1)$. It is clear that the second term on the right-hand side of Eq. (9) gives the corrections due to the effect of finite number of particles. In deriving the expression of mean occupation numbers, Eq. (9), the approximation holds well when N is not very small, indicating that this approach is not exactly for the finite systems. However, this approach has the merit of being very simple for calculation, without sacrifice of physical illumination.

3. Specific heat and condensation fraction

In a 3D harmonic potential, the energy spectrum is $\epsilon_v = \hbar\omega \sum_{i=1}^{3} v_i$ ($v_i = 0,\ 1,\ 2,\ \ldots$) which, for the isotropic case, is equivalent to

$$\epsilon_m = m\hbar\omega, (m = 0,\ 1,\ 2,\ \ldots) \qquad (10)$$

with a multiplicity factor $g_m = (m+1)(m+2)/2$ accounting for the degeneracy of the single-particle states with ϵ_m. For a fixed number N of particles, the chemical potential can be calculated by the following constraint

$$N = \sum_m g_m n_m(\epsilon_m). \qquad (11)$$

The average energy E_N of the system is determined by

$$E_N = \sum_{m=0}^{\infty} g_m n_m(\epsilon_m)\epsilon_m. \qquad (12)$$

Here $\langle n_m \rangle$ denoted in Eq. (9) is the mean occupation number in each of the energy level ϵ_m. The number of particles in the condensate ($\epsilon_0 = 0$) is given by the $m = 0$ term of expression (9):

$$n_0 = \frac{1}{\mathrm{e}^{-\beta\mu} - 1} - \frac{N+1}{\mathrm{e}^{-(N+1)\beta\mu} - 1}. \qquad (13)$$

From Eqs. (10) and (12), the specific heat C_N at fixed N can be straightforwardly calculated, and the result is

$$C_N = \beta \sum_m \left[\frac{g_m \epsilon_m \mathrm{e}^{\beta(\epsilon_m-\mu)}}{\mathrm{e}^{\beta(\epsilon_m-\mu)}-1} - \frac{g_m (N+1)^2 \epsilon_m \mathrm{e}^{(N+1)\beta(\epsilon_m-\mu)}}{\mathrm{e}^{\beta(N+1)(\epsilon_m-\mu)}-1} \right] \left(\frac{\epsilon_m - \mu}{T} + \frac{\partial \mu}{\partial T} \right), \tag{14}$$

where $\partial\mu/\partial T$ can be got by differentiating Eq. (11) with respect to T

$$\frac{\partial \mu}{\partial T} = \frac{\sum_{m=0}^{\infty} g_m (\epsilon_m - \mu) \mathrm{e}^{\beta(\epsilon_m-\mu)} [\eta^2(\epsilon_m) - \eta_N^2(\epsilon_m) \mathrm{e}^{N\beta(\epsilon_m-\mu)}]}{T \sum_{j=0}^{\infty} g_j \mathrm{e}^{\beta(\epsilon_j-\mu)} [\eta^2(\epsilon_j) - (N+1)^2 \eta_N^2(\epsilon_j) \mathrm{e}^{N\beta(\epsilon_j-\mu)}]}, \tag{15}$$

with $\eta(\epsilon_m) = 1/(\mathrm{e}^{\beta(\epsilon_m-\mu)}-1)$ and

$$\eta_N(\epsilon_m) = \frac{N+1}{\mathrm{e}^{(N+1)\beta(\epsilon_m-\mu)}-1}.$$

The use of Eqs. (10)–(15) allows us to find the thermodynamic properties of the 3D harmonic trapped finite Bose gas. Now, we are in a position to do numerical calculations. From Eq. (11) we calculate the chemical potential μ as a function of temperature T and particle number N. In Fig. 1 we have shown, for different

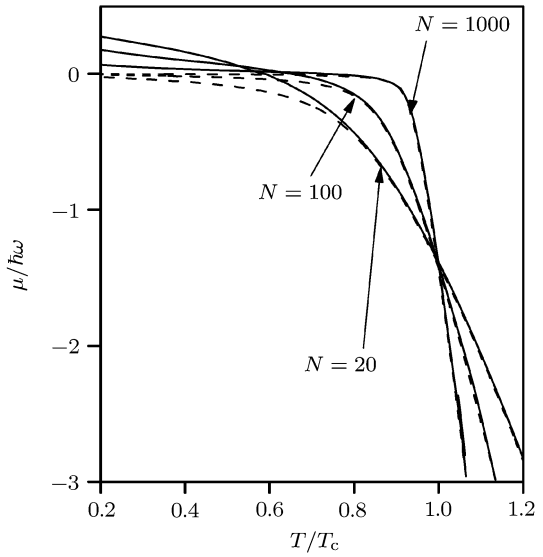


Fig. 1. The chemical potential μ in unit of $\hbar\omega$ versus temperature T in unit of T_c^0, the critical temperature in the thermodynamic limit. The system consists of N ($N = 20, 100, 1000$) ideal bosons confined in the 3D isotropic harmonic potential. Solid lines are our results computed from Eq. (11). Dashed lines are corresponding ones in the grand canonical ensemble.

N, the chemical potential in unit of the harmonic energy $\hbar\omega$ as a function of temperature in unit of the transition temperature

$$T_c^0 = \left(\frac{N}{\zeta(3)} \right)^{1/3} \frac{\hbar\omega}{k_B}$$

in the thermodynamic limit. In the figure, the solid (dashed) lines are computed from Eq. (11) (from the corresponding equation in the grand canonical ensemble). From the figure we see that there are several interesting features for the chemical potential. First, we have $\mu \geq 0$ (solid lines) at sufficiently low temperatures. This originates from the properties of the distribution law in Eq. (9) $n(u) = 1/(\mathrm{e}^u - 1) - (N+1)/[\mathrm{e}^{(N+1)u} - 1]$ with $u = \beta(\epsilon_m - \mu)$: the function $n(u)$ is (a) positive and (b) monotonically decreasing from $n(-\infty) = N$ through $n(0) = N/2$ to $n(\infty) = 0$ (see Appendix A in Ref. [15] for the detail). While we have $\mu \leq 0$ (dashed lines) in the grand canonical calculations for all temperatures T due to the ordinary Bose statistics. Second, at sufficiently low temperatures the chemical potential μ decreases (increases) as the particle number N increases in our (grand canonical) calculations. Third, the difference of chemical potential between ours and grand canonical calculations becomes small with increasing particle numbers.

From Eqs. (14) and (15) we calculate the specific heat C_N as a function of temperature T and particle number N. In Fig. 2 is shown the specific heat in unit of Nk_B as a function of temperature in unit of the transition temperature T_c^0 for different N. As mentioned above, the transition temperature T_c can be defined as the point corresponding to the maximum value of the specific heat for finite systems, i.e., $\partial C_N(T)/\partial T|_{T=T_c} = 0$.[12] In the figure, the solid (dashed) lines are our (grand canonical) results. We note that finite-size effect produces some shift of the transition temperature T_c toward value lower than T_c^0. From the figure we also see the specific heat shows humps and peaks at about $T = T_c(N)$ for finite and large enough N, respectively. The smooth humps change to sharp peaks as N increases. For fixed and small N, the difference of specific heats between our and grand canonical calculations is visible for temperatures lower than the transition temperature $T_c(N)$. As expected, the specific heats in our calculation are substantially in excellent agreement with those in the grand canonical ensemble[12,15] for large enough N.

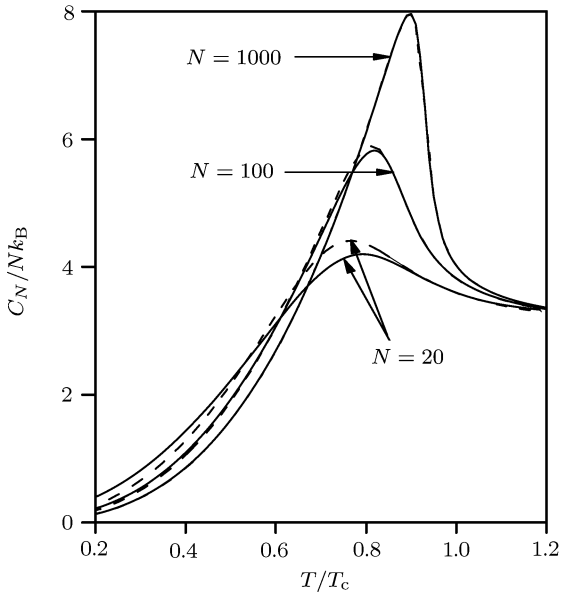


Fig. 2. The specific heat per particle in unit of k_B versus temperature T in unit of T_c^0, the transition temperature in the thermodynamic limit. The system consists of N ($N = 20, 100, 1000$) ideal bosons confined in the 3D isotropic harmonic potential. Solid lines are our results computed from Eq. (14). Dashed lines are corresponding ones in the grand canonical ensemble.

From Eqs. (11) and (13) we calculate the condensate fraction n_0/N as a function of temperature T and particle number N. In Fig. 3 it is shown the condensate fraction as a function of temperature in unit of the critical temperature T_c^0 for different N. For fixed and small N, the maximum difference of condensate fractions between our and grand canonical calculations is in the middle region between 0 and $T_c(N)$. The drop of condensate fraction at low temperatures becomes large with increasing N.

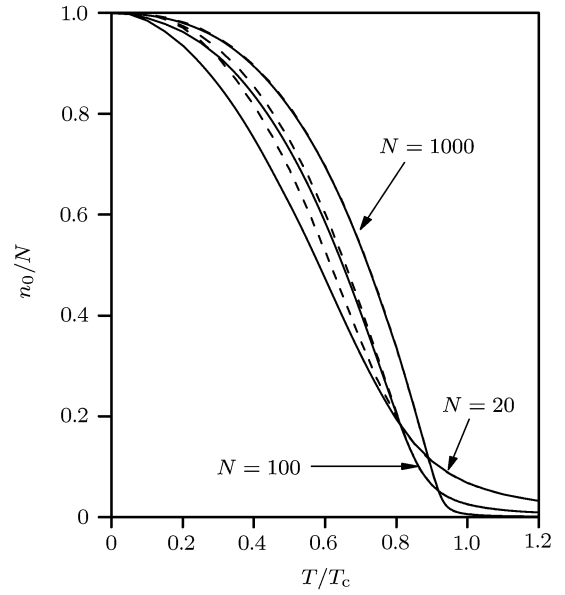


Fig. 3. The condensate fraction versus temperature in unit of T_c^0, the transition temperature in the thermodynamic limit. The system consists of N ($N = 20, 100, 1000$) ideal bosons confined in the 3D isotropic harmonic potential. Solid lines are our results computed from Eq. (13). Dashed lines are corresponding ones in the grand canonical ensemble.

Now we investigate the finite-size scaling behaviour of the condensate fraction of the 3D ideal Bose gas in the harmonic trap. The central assumption of finite-size scaling is that at the critical region all physical quantities scale as functions of the correlation length ξ to the system size L. According to the scaling properties of the condensate fraction n_0/N (or the related superfluid density),[51−53,45] near the transition point T_c the thermodynamical quantities in finite systems will depend on temperature T and particle number N only through the ratio of a characteristic system size L to the bulk correlation length $\xi(t)$ with $t = (T - T_c)/T_c$. That means if $n_0/N \sim t^\phi$ with ϕ being the condensate fraction exponent then its finite-size behaviour obeys the scaled form

$$n_0(t, L)/N = L^{-\phi/\nu} Q[(L/\xi(t))^{1/\nu}], \qquad (16)$$

where $\xi(t) \sim t^{-\nu}$ with ν being the correlation length exponent and

$$Q(tL^{1/\nu}) = Q(0) + qtL^{1/\nu} \qquad (17)$$

with $Q(0)$ and q being constants. Since $\phi = \nu$[51−53,45] and $L \sim N^{1/6}$ for the trapped case, the scaled form in our case becomes $\langle n_0(t, N)\rangle/N^{5/6} = Q_0 + q_0 t N^{1/6\nu}$. Our numerical results show that $Q_0 = 0.356 \pm 0.005$ is an universal constant and $q_0 = -0.704 \pm 0.023$. The scaled data and the resulting linear fit are plotted in Fig. 4. The best-fit parameter is the correlation length exponent $\nu = 0.55 \pm 0.14$. The fitted solid line in Fig. 4 shows that the condensate fractions for various system sizes and temperatures collapse onto a single form for an ideal Bose gas in a 3D isotropic harmonic trap. For a noninteracting gas the critical exponent can be exactly calculated by renormalization group method with $\nu = 1$ for homogeneous systems and $\nu = 1/2$ for harmonically trapped systems. (For a weakly interacting trapped Bose gas, the measured value is $\nu = 0.67 \pm 0.13$.[56]) Therefore, our result $\nu = 0.55 \pm 0.14$ agrees well with the exact theoretical value $\nu = 0.5$, which supplies a strong argument in favour of our approach.

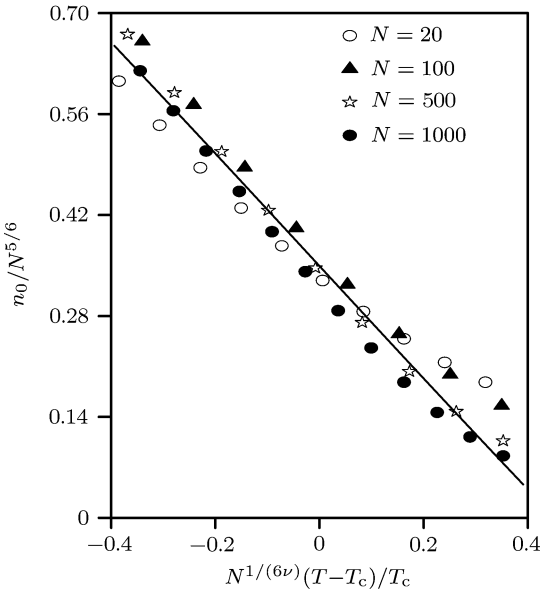


Fig. 4. The scaled condensate fraction versus scaled temperature.

4. Conclusions

We have derived the simple analytical expression for the mean occupation number in any state for the finite-size noninteracting Bose systems. We have investigated the various thermodynamical quantities for the finite Bose systems. Comparing these results with those in the grand canonical ensemble, there is a quantitative or even qualitative difference at sufficiently low temperatures, specially for small systems. The finite-size effects described above are visible, particularly in the case when the temperatures are sufficiently low.

A nice feature of this work is that the analysis of BEC with a finite number of particles is performed in consideration of conservation of the total number of particles N. It is therefore more suitable to discuss the BEC with a finite number of particles. We have presented the finite-size scaling analysis for various system sizes, which shows the universal law of the systems at the transition point. We can approach the BEC systems with any particle numbers or even only several particles to explore some novel physics. Since we have the simple analytical results for the thermodynamic properties, our subsequent work will be to apply this method to study the interacting trapped Bose systems with finite number of particles.

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