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Bose gases in one-dimensional harmonic trap

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Abstract. Thermodynamic quantities, occupation numbers and their fluctuations of a one-dimensional Bose gas confined by a harmonic potential are studied using different ensemble approaches. Combining number theory methods, a new approach is presented to calculate the occupation numbers of different energy levels in microcanonical ensemble. The visible difference of the ground state occupation number in grand-canonical ensemble and microcanonical ensemble is found to decrease by power law as the number of particles increases.

Keywords. Bose gas; occupation number; ensemble theory.

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1. Introduction

Due to the experimental realization of Bose–Einstein condensation (BEC) in the year 1995 [1–3], Bose system at low temperature became a research hotspot in physics. The interaction between the particles in optical trap can be easily adjusted by Feshbach resonance technique [4,5]. Therefore, BEC becomes a clean object to test various theories. Moreover, the number of trapped particles is not up to the macroscopic level, and so finite number effect can be observed in this system. Trapped Bose system can exhibit many thermodynamic phenomena.

A discipline called quantum thermodynamics [6], which generalizes classical thermodynamics concepts to quantum region, was developed in recent years to describe the thermodynamic properties of the microscopic systems. Both heat and work of a quantum system depend on the occupation numbers of different energy levels of the system [7]. As a candidate of the working substance of quantum heat engine, the occupation number of the BEC system is worth studying carefully.

For cold gases of neutral Bose atoms trapped in optical cavities, due to the atomic number conservation and weak coupling with the environment, microcanonical ensemble approach can be applied. Recently, BEC of a two-dimensional photon gas was realized in a dye microcavity [8], in which photons were frequently absorbed and emitted by the dye molecules. The dye molecules served as both heat bath and particle reservoir, and so the photon gas satisfied grand-canonical conditions [9]. For convenience, BEC systems are usually studied using grand-canonical ensemble. However, it is necessary to use different ensembles due to different physical conditions.

Fluctuation in a low-temperature system is a matter of controversy in physics [10,11]. It is well known that the grand-canonical treatment loses its validity when there is a fluctuation of occupation number of the quantum system [12,13]. The fluctuation of occupation number of extreme relativistic particles in grand-canonical ensemble could be measured precisely so far [9]. Thus, the fluctuation of occupation number of the BEC system is also discussed in this paper.

If two dimensions of the three-dimensional asymmetric optical cavity which is used to trap Bose atoms are tight-bonded and no particle can be excited in these two dimensions, the system becomes quasi-one-dimensional. Bose systems trapped in one-dimensional potential have attracted wide interest [12–20].

2. Grand-canonical ensemble

Consider an ideal Boson system trapped in one-dimensional harmonic trap with energy level spacing

ε. For convenience, the ground-state energy level is set to be potential energy zero. The system can exchange energy and particles with the heat bath in grand-canonical ensemble. If the temperature and chemical potential of the system are T and μ, the expectation of the occupation number of the ith energy level is

$$\langle n_i \rangle = \frac{1}{\exp[(i\varepsilon - \mu)/kT] - 1}, \tag{1}$$

where $i = 0, 1, 2, 3, \ldots$ and k is the Boltzmann constant. The total number of particles and total energy of the system can be determined by equations

$$\langle N \rangle = \sum_i \langle n_i \rangle, \tag{2}$$

$$\langle E \rangle = \sum_i i\varepsilon \langle n_i \rangle. \tag{3}$$

The fluctuations of the occupation numbers are not only due to the transitions among different energy levels but also due to the particle exchange with the heat bath. The fluctuation of any given energy level $\delta n_i^2 \equiv \langle n_i^2 \rangle - \langle n_i \rangle^2$ can be obtained by the following equation [21]:

$$\frac{\delta n_i^2}{\langle n_i \rangle^2} = \frac{1}{\langle n_i \rangle} + 1. \tag{4}$$

Most particles will condense to the ground state when the temperature gets close to zero. At this time $\langle n_0 \rangle$ and $\langle N \rangle$ have the same order of magnitude, and thus the fluctuation of the ground-state population δn_0 becomes comparable with the total number of particles $\langle N \rangle$ based on eq. (4). This is because the thermal wavelengths of particles exceed the size of the system at low temperature, and thus the boundary between the system and the bath becomes ambiguous; rather, bath loses its specific physical meaning at this time.

3. Microcanonical ensemble

The number of particles N and the total energy of the system are conserved in microcanonical ensemble. Different combination of occupations $\{n_0, n_1, n_2, \ldots\}$ which satisfies the microcanonical conditions

$$\begin{cases} \sum_{i=0}^{\infty} n_i = N \\ \sum_{i=0}^{\infty} i n_i = m \end{cases} \tag{5}$$

corresponds to different microstates. The integer m in eq. (5) is the number of excitation quanta $m \equiv E/\varepsilon$. The problem of counting the number of microstates can be transferred to the problem of partitions of positive integer if $m \leq N$. For example, for $m = 3 \leq N$ there are three partitions, i.e., $m = 3$, $m = 2+1$ and $m = 1+1+1$, corresponding to three different bosonic microstates $\{N-1, 0, 0, 1, 0, 0, \ldots\}$, $\{N-2, 1, 1, 0, 0, \ldots\}$ and $\{N-3, 3, 0, 0, \ldots\}$. The problem to determine the partition number $p(m)$ of a given integer m was first proposed by Andrews in [22]. Rademacher gave exact expression of $p(m)$ in the year 1937 [23]. When $m > N$, the possible partition number $p_N(m)$ is less than $p(m)$ due to the restriction of the number of particles. For example, for $m = 3$, $N = 2$, there are only two partitions, $m = 3$ and $m = 2 + 1$, corresponding to two different bosonic microstates $\{1, 0, 0, 1, 0, 0, \ldots\}$ and $\{0, 1, 1, 0, 0, \ldots\}$.

The exact expression of $p(m)$ is very complex. Yet, Hardy and Ramanujan [24] gave the asymptotic formula of $p(m)$ as

$$p(m) \sim \frac{\exp\left(\pi\sqrt{(2/3)m}\right)}{4\sqrt{3}m}. \tag{6}$$

The defect of eq. (6) is that it diverges when $m \to 0$. To make the expression of $p(m)$ more suitable for our calculation, we rewrite eq. (6) as

$$p(m) \approx \frac{\exp\left(\pi\sqrt{(2/3)m}\right)}{4\sqrt{3}(m+1)}. \tag{7}$$

From figure 1, it can be seen that eq. (7) works better than eq. (6) especially when m is not large.

Erdos and Lehner [25] gave the approximate expression of $p_N(m)$

$$p_N(m) \approx p(m) \exp\left[-\frac{\sqrt{6m}}{\pi} \exp\left(-\frac{\pi}{\sqrt{6}}\frac{N}{\sqrt{m}}\right)\right]. \tag{8}$$

From eq. (8), for $\sqrt{m} \ll N$ we have $p_N(m) \approx p(m)$.

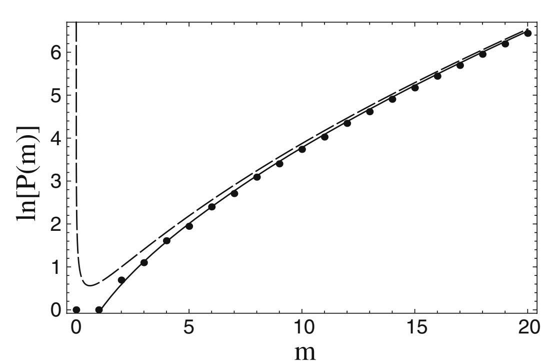

Figure 1. The value of $p(m)$. (•) Exact value, (—) the result of eq. (7) and (- - -) the result of eq. (6).

The entropy of the system can be directly derived from the number of microstates $p_N(m)$

$$S = k \ln[p_N(m)]. \tag{9}$$

Then the temperature of the system is

$$T = \frac{1}{(\partial S/\partial E)_N}. \tag{10}$$

If one uses the exact value of $p_N(m)$ instead of the approximate value, the partial derivative in eq. (10) should be replaced by

$$T(N,m) = \frac{E(N,m+1) - E(N,m-1)}{S(N,m+1) - S(N,m-1)}.$$

All the microcanonical results for $N = 10$ are derived using the exact value of $p_N(m)$ and the difference. From this discussion, it is easy to show a quadratic functional relationship between the energy and the temperature for $1 \ll \sqrt{m} \ll N$

$$m = \frac{E}{\varepsilon} = \frac{\pi^2}{6}\left(\frac{kT}{\varepsilon}\right)^2. \tag{11}$$

The expectation value of the occupation number $\langle n_i \rangle$ can be obtained as an average over n_i of each possible microstate when m and N are not large, and the fluctuation of occupation number δn_i can also be obtained using this method. The microcanonical results for $N = 10$ are counted out from these finite microstates. However, this method is not suitable for large m and N because the number of microstates grows exponentially with m and N. Using the number theory results of Auluck *et al* [26], Grossmann and Holthaus [12] derived the statistical weight of different n_0 for given m and N, hence obtained $\langle n_0 \rangle$ and δn_0. We use another simple and effective method to deduce the occupation number and its fluctuation. Suppose n_0 bosons are occupying the ground state. Then eq. (5) can be rewritten as

$$\begin{cases} \sum_{i=0}^{\infty} n_{i+1} = N - n_0 \\ \sum_{i=0}^{\infty} i n_{i+1} = m - N + n_0 \end{cases}. \tag{12}$$

Equations (12) and (5) are equivalent mathematically, but the number of solutions for eq. (12) is $p_{N-n_0}(m - N + n_0)$ for fixed n_0. To guarantee $p_{N-n_0}(m - N + n_0)$ is well defined, it should satisfy the condition $N - m \le n_0 \le N$. Since different solutions correspond to different microstates, the statistical weight of the occupation number of the ground state is

$$w_0(n_0) = \frac{p_{N-n_0}(m - N + n_0)}{\sum_{n_0'=N-m}^{N} p_{N-n_0'}(m - N + n_0')}. \tag{13}$$

The statistical weight can be obtained by inserting eqs (7) and (8) into eq. (13). Figure 2 shows that the weight we obtain coincides with that derived by Grossmann and Holthaus. The deviation between our weight and the weight given by Grossmann and Holthaus is small for $N = 100$ and $N = 1000$ and decreases with the increase of N. We have checked the case of $N = 10^6$ and found that there is no detectable difference between these two methods.

The occupation number and its fluctuation of the ground state can be obtained by

$$\langle n_0 \rangle = \sum_{n_0'=N-m}^{N} n_0' w_0(n_0'), \tag{14}$$

$$\delta n_0^2 = \sum_{n_0'=N-m}^{N} n_0'^2 w_0(n_0') - \langle n_0 \rangle^2. \tag{15}$$

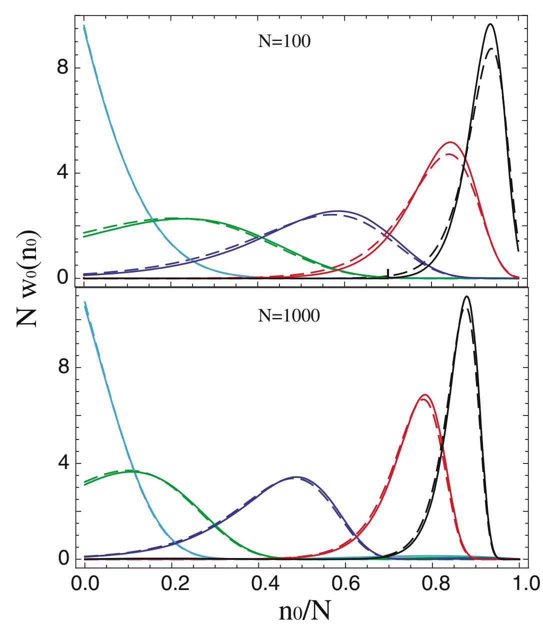

Figure 2. The statistical weight $w_0(n_0)$ of different n_0 for given m and N. (—) The results of our method eq. (13), (- - -) the results of Grossmann and Holthaus [12]. Top: $N = 100$, cyan, green, blue, red and black represent $m = 3000, 1000, 400, 100, 30$ respectively. Bottom: $N = 1000$, cyan, green, blue, red and black represent $m = 80000, 50000, 20000, 5000, 2000$ respectively.

Here we take $\langle n_1\rangle$ as an example to demonstrate the method to calculate the occupation number of other energy levels. Equations (5) and (12) can be rewritten equivalently as

$$\begin{cases} \sum_{i=0}^{\infty} n_{i+2} = N - n_0 - n_1 \\ \sum_{i=0}^{\infty} i n_{i+2} = m - 2N + 2n_0 + n_1 \end{cases}. \tag{16}$$

For given n_0 and n_1, the number of solutions for eq. (16) is $p_{N-n_0-n_1}(m - 2N + 2n_0 + n_1)$, where $2N - 2n_0 - m \le n_1 \le N - n_0$. Therefore, for a given n_0, the statistical weight of n_1 particles occupying the first excited state is

$$w_1(n_1|n_0) = \frac{p_{N-n_0-n_1}(m - 2N + 2n_0 + n_1)}{\sum_{n_1'=2N-2n_0-m}^{N-n_0} p_{N-n_0-n_1}(m-2N + 2n_0 + n_1')}. \tag{17}$$

Hence, expectation value of the occupation number of the first excited state is

$$\langle n_1\rangle = \sum_{n_0'=N-m}^{N} \sum_{n_1'=2N-2n_0'-m}^{N-n_0'} n_1' w_1(n_1'|n_0') w_0(n_0'). \tag{18}$$

The double summations in eq. (18) are impractical. As an approximation, the fluctuation of n_0 can be ignored and we use $\langle n_0\rangle$ of eq. (14) to replace n_0. Then eq. (18) becomes

$$\langle n_1\rangle = \sum_{n_1'=2N-2\langle n_0\rangle-m}^{N-\langle n_0\rangle} n_1' w_1(n_1'|\langle n_0\rangle). \tag{19}$$

For convenience, the summations in eqs (14), (15), (19) can be replaced by integrations for large N.

The same procedure can be used to calculate expectation values of the occupation numbers of other energy levels: By ignoring the fluctuations of $n_0, n_1, \ldots, n_{i-1}$, the statistical weight $w_i(n_i|\langle n_0\rangle, \langle n_1\rangle, \ldots, \langle n_{i-1}\rangle)$ can be calculated and hence $\langle n_i\rangle = \sum_{n_i'} n_i' w_i(n_i|\langle n_0\rangle, \langle n_1\rangle, \ldots, \langle n_{i-1}\rangle)$.

4. Canonical ensemble

In canonical ensemble, the system can exchange energy with the heat bath. The probability that a certain microstate $\{n\} \equiv \{n_0, n_1, \ldots, n_i, \ldots \mid \sum_i n_i = N\}$ will occur depends on the energy of the microstate $E(\{n\}) = \varepsilon \sum_i i n_i$ and the temperature T of the heat bath

$$\rho(\{n\}) \sim \exp\left[-\frac{E(\{n\})}{kT}\right]. \tag{20}$$

From the previous section, it is known that there are $p_N(m)$ microstates corresponding to the same energy εm in the system. Thus, the average energy of the system is

$$\langle E\rangle = \frac{\sum_m \varepsilon m p_N(m) \exp(-\varepsilon m/kT)}{\sum_m p_N(m) \exp(-\varepsilon m/kT)}. \tag{21}$$

By using the conclusion of the number theory, Herzog and Olshanii [16] gave the average occupation number in canonical ensemble as

$$\langle n_i\rangle = \sum_{j=1}^{N} x^{(N-j+1)i} \prod_{q=j}^{N} (1 - x^q), \tag{22}$$

where $x = \exp(-\varepsilon/kT)$.

5. Results and discussion

Grossmann and Holthaus [12] showed that the trapped Bose gas in harmonic potential has a characteristic temperature

$$T_0 = \frac{\varepsilon}{k}\frac{N}{\ln N}, \tag{23}$$

below which most of the particles occupy the ground state. However, various physical quantities do not exhibit any abrupt change and there is no phase transition in the vicinity of the characteristic temperature.

The energy–temperature curves obtained in different ensembles are shown in figure 3. It is clear that the results given by different ensembles are visibly different for few-body systems, and the differences among these ensembles decrease with the increase in the number of particles. From eq. (11), if the horizontal axis and the vertical axis change to T/T_0 and $(\ln N/N)^2\,(E/\varepsilon)$ respectively, all the curves will overlap together approximately. However, it will be difficult to see the tendency of changing number of particles by doing so. Therefore, we use the horizontal axis and the vertical axis in figure 3. Note that the microcanonical results for $N = 10$ are exact and all are derived by finding all the possible microstates using computer simulations.

Figure 4 shows the relationship between the occupation number of the ground state and the temperature in

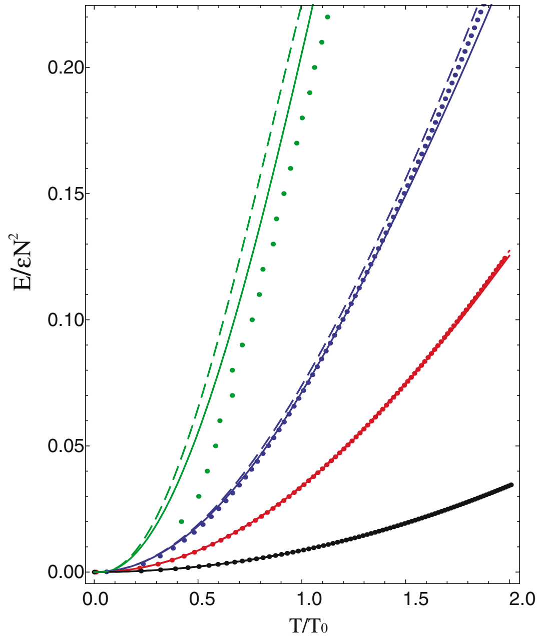

Figure 3. The energy–temperature curves obtained in different ensembles. (—) Grand-canonical ensemble, (- - -) canonical ensemble and (•) microcanonical ensemble. Green, blue, red and black represent $N = 10, 100, 1000, 10^6$ respectively.

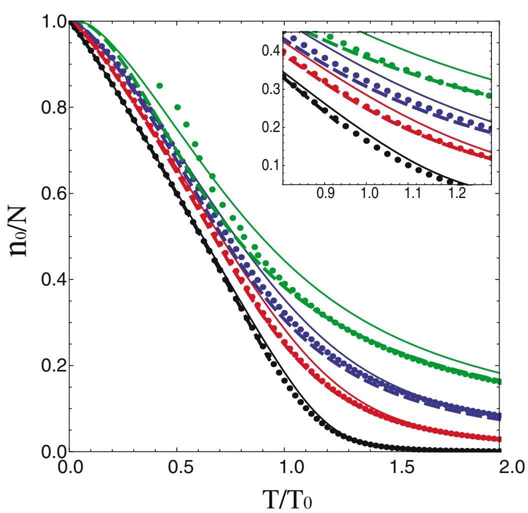

Figure 4. Ground-state fraction as a function of temperature. (—) Grand-canonical ensemble, (- - -) canonical ensemble and (•) microcanonical ensemble. Green, blue, red and black represent $N = 10, 100, 1000, 10^6$ respectively.

different ensembles. The results from the microcanonical ensemble and the canonical ensemble agree with each other very well, and there is no visible difference between them for $N > 1000$. However, the results from the grand-canonical ensemble differ from the results from the other two ensembles even when the number of particles reaches 10^6.

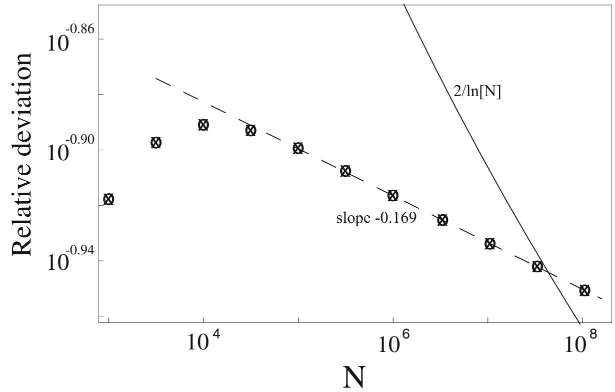

Figure 5. The relative deviation of the ground-state fraction between the grand-canonical ensemble and the microcanonical ensemble $(\langle n_0^{\text{gr. canon.}}\rangle - \langle n_0^{\text{mic. canon.}}\rangle)/\langle n_0^{\text{mic. canon.}}\rangle$ as a function of the number of particles N. (◯) the results given by our method and (×) the results given by the method proposed by Grossmann and Holthaus. We draw the solid line of $2/\ln N$ for comparison.

Herzog and Olshanii [16] once calculated the relative deviation between grand-canonical ensemble and canonical ensemble $(\langle n_0^{\text{gr. canon.}}\rangle - \langle n_0^{\text{canon.}}\rangle)/\langle n_0^{\text{canon.}}\rangle$. They believe that this relative deviation decays with the number of particles N as a scale of $1/\ln N$ for fixed T/T_0. Here, we calculate the relative deviation between grand-canonical ensemble and microcanonical ensemble $(\langle n_0^{\text{gr. canon.}}\rangle - \langle n_0^{\text{mic. canon.}}\rangle)/\langle n_0^{\text{mic. canon.}}\rangle$ at $T = T_0$. For microcanonical ensemble, we obtain the results by using not only our method given in §3 but also the method proposed by Grossmann and Holthaus. Both these methods show that the relative deviation between the grand-canonical ensemble and the microcanonical ensemble decreases as $N^{-0.169}$ other than $1/\ln N$ (see figure 5). As there is no difference between the ground-state fraction given by the microcanonical ensemble and the ground-state fraction given by the canonical ensemble for $N > 1000$, we do not agree with the conclusion given by Herzog and Olshanii. The relative deviation between the grand-canonical ensemble and other ensembles decays very slowly with N because 0.169 is a very small power exponent. For example, the relative deviation is 11.7% when $N = 10^7$, and the relative deviation is still 6.3% when the system reaches the macroscopic level 10^{23}.

Figure 6 shows the relationship between the ground-state fluctuation and the temperature in both microcanonical ensemble and grand-canonical ensemble. In grand-canonical ensemble, the fluctuation of the ground-state fraction increases monotonically as temperature decreases, and the fluctuation of the occupation number of the ground state becomes comparable

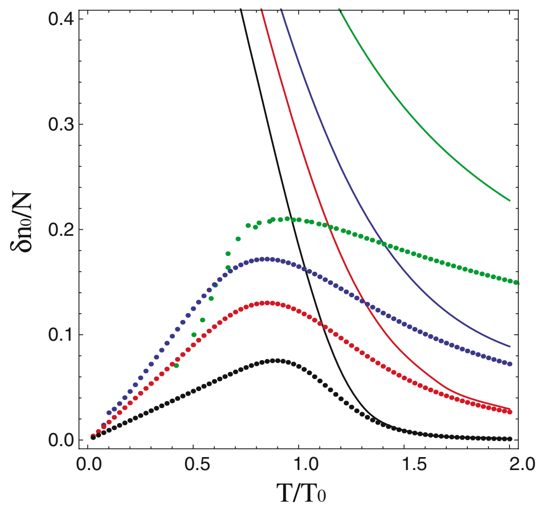

Figure 6. The relationship between the ground-state fluctuation and the temperature in both microcanonical ensemble and grand-canonical ensemble. (—) Grand-canonical ensemble and (•) microcanonical ensemble. Green, blue, red and black represent $N = 10, 100, 1000, 10^6$ respectively.

with the total number of particles in this system when $T < T_0$. The fluctuations in these two different ensembles coincide with each other when $T \gg T_0$. On the contrary, the fluctuation in microcanonical ensemble decreases as the temperature decreases when $T < T_0$ and vanishes at $T = 0$.

The occupation numbers of the first excited state in various ensembles are shown in figure 7. The occupation numbers of the first excited state increase with temperature when $T < T_0$, reach the maximum around T_0 and then decrease with temperature.

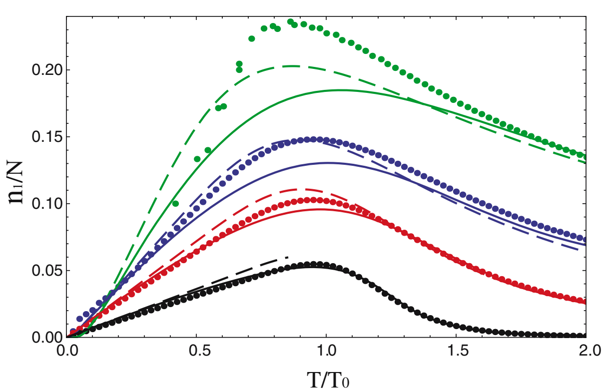

Figure 7. The occupation numbers of the first excited state in various ensembles. (—) Grand-canonical ensemble, (- - -) canonical ensemble and (•) microcanonical ensemble. Green, blue, red and black represent $N = 10, 100, 1000, 10^6$ respectively.

6. Conclusion

We have presented an intensive study on ideal bosons trapped in harmonic potential. The results calculated using different ensembles are compared in detail. In microcanonical ensemble, we derived the statistical weight of the occupation number of a given energy level by adopting the results of partition theory, and obtained the expected value and the fluctuation of the occupation number. We found that the thermodynamic quantities given by the microcanonical ensemble and the grand-canonical ensemble are almost equal when N is larger than 1000 while the ground-state occupation numbers given by these two ensembles still have visible deviation. We have found that this deviation decreases according to a power law with the number of particles with the exponent -0.169.

Acknowledgements

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References

[1] M H Anderson, J R Ensher, M R Matthews, C E Wieman and E A Cornell, *Science* **269**, 198 (1995)
[2] K B Davis, M O Mewes, M R Andrews, N J van Druten, D S Durfee, D M Kurn and W Ketterle, *Phys. Rev. Lett.* **75**, 3969 (1995)
[3] C C Bradley, C A Sackett, J J Tollett and R G Hulet, *Phys. Rev. Lett.* **75**, 1687 (1995)
[4] E Timmermans, P Tommasini, M Hussein and A Kerman, *Phys. Rep.* **315**, 199 (1999)
[5] R A Duine and H T C Stoof, *Phys. Rep.* **396**, 115 (2004)
[6] J Gemmer, M Michel and G Mahler, *Quantum thermodynamics* (Springer, Berlin, 2004)
[7] T D Kieu, *Phys. Rev. Lett.* **93**, 140403 (2006)
[8] J Klaers, J Schmitt, F Vewinger and M Weitz, *Nature* **468**, 545 (2010)
[9] J Schmitt, T Damm, D Dung, F Vewinger, J Klaers and M Weitz, *Phys. Rev. Lett.* **112**, 030401 (2014)
[10] J X Hou, X Wang, S Huang, J J Lin, C L Wang and Q H Liu, *Acta Phys. Sin.* **55**, 1616 (2006)
[11] T C P Chui, D R Swanson, M J Adriaans, J A Nissen and J A Lipa, *Phys. Rev. Lett.* **69**, 3005 (1992)
[12] S Grossmann and M Holthaus, *Phys. Rev. E* **54**, 3495 (1996)

[13] M Holthaus, E Kalinowski and K Kirsten, *Ann. Phys.* **270**, 198 (1998)
[14] V Bagnato and D Kleppner, *Phys. Rev. A* **44**, 7439 (1991)
[15] W Ketterle and N J van Druten, *Phys. Rev. A* **54**, 656 (1996)
[16] C Herzog and M Olshanii, *Phys. Rev. A* **55**, 3254 (1997)
[17] J Catani, G Barontini, G Lamporesi, F Rabatti, G Thalhammer, F Minardi, S Stringari and M Ingusci, *Phys. Rev. Lett.* **103**, 140401 (2009)
[18] J X Hou, *Phys. Lett. A* **368**, 366 (2007)
[19] G Q Li, L B Fu, J K Xue, X Z Chen and J Liu, *Phys. Rev. A* **74**, 055601 (2006)
[20] J X Hou, *J. Low Temp. Phys.* **177**, 305 (2014)
[21] R K Pathria, *Statistical mechanics* (Butterworth-Heinemann, Singapore, 1996)
[22] G E Andrews, *The theory of partitions* (Addison-Wesley, Reading, 1976)
[23] H Rademacher, *Proc. Natl Acad. Sci.* **23**, 78 (1937)
[24] G H Hardy and S Ramanujan, *Proc. London Math. Soc.* **17**, 75 (1918)
[25] P Erdos and J Lehner, *Duke Math. J.* **8**, 335 (1941)
[26] F C Auluck, S Chowla and H Gupta, *J. Ind. Math. Soc.* **6**, 105 (1942)