

# Thermodynamic Properties of Bosons in Symmetric Double-well Potentials

J. Choy, K. L. Liu, C. F. Lo, and F. So

Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong

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We study the thermodynamic properties and the Bose-Einstein condensation (BEC) for a finite number  $N$  of identical non-interacting bosons in the field of a deep symmetric double-well potential (SDWP). The temperature dependence of the heat capacity  $C(T)$  at low temperatures is analyzed, and we derive several generic results which are valid when the energy difference between the first two excited states is sufficiently large. We also investigate numerically the properties of non-interacting bosons in three-dimensional superpositions of deep quartic SDWP's. At low temperatures, we find that  $C(T)$  displays microstructures which are sensitive to the value of  $N$  and the thermal variation of the condensate fraction shows a characteristic plateau. The origin of these features is discussed, and some general conclusions are drawn.

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## 1. Introduction

Recently, the Bose-Einstein condensation (BEC) has been realized in magnetically trapped alkali atomic gases at ultracold temperatures [1–4]. This experimental achievement has stimulated intense interest in the physics of a confined inhomogeneous Bose gas consisting of a limited number  $N$  of bosons ( $10^3 \leq N \leq 10^7$ ). As the experiments deal with dilute atomic gases and the typical magnetic traps can be modelled by harmonic oscillator potentials [5, 6], considerable theoretical efforts have been made to understand the thermodynamic properties of a mesoscopic ideal Bose gas moving in such potential fields [7–13]. It is now well appreciated that the presence of a confining potential, in conjunction with the constraint of a finite  $N$ , has profound effects on the BEC, especially for low-dimensional systems [8, 12]. For example, for highly anisotropic harmonic traps, it has been shown that a novel two-step condensation can take place [13], which arises from the great disparity in the energy-level spacings of the single-particle quantum states associated with the different confining dimensions. Motivated by this interesting finding, we shall study in this work the BEC of an ideal Bose gas in the field of a symmetric double-well potential. The more complicated effects due to a three-dimensional superposition of symmetric double-well potentials will be examined also.

Owing to the quantum tunneling effect, the single-particle eigenenergy spectrum of the low-lying excited states of a symmetric double-well potential consists of a series of doublets, each one composed of two closely spaced energy levels [14]. For deep potential wells, the energy difference  $\Delta = (E_1 - E_0)$  between the first excited state and the ground state is minute in comparison with the energy gap  $G = (E_2 - E_1)$  between the first two excited states. For example, in the case of the one-dimensional potential  $V(8; x) = \hbar\omega \times (-8x^2 + x^4)$ , where  $x$  is a dimensionless co-ordinate and the constant  $\hbar\omega$  sets the energy scale, we have  $\Delta = 1.6 \times 10^{-5} \hbar\omega$  and  $(G/\Delta) = 3.3 \times 10^5$ , while the potential  $V(10; x)$  gives  $\Delta = 5.0 \times 10^{-8} \hbar\omega$  and  $(G/\Delta) = 1.2 \times 10^8$ . The fact that the ratio  $(G/\Delta)$  can be exponentially large [14] has important thermodynamic consequences for a bosonic system. When a finite number  $N$  of identical non-interacting bosons are distributed among such single-particle states according to the Bose-Einstein statistics, the low-temperature thermodynamic properties of the system depend sensitively on the energy ratio  $(G/N\Delta)$ . A system with  $G > N\Delta$  will be referred to as a wide-gap system, while the case with  $G < N\Delta$  will be called a narrow-gap system. For a wide-gap system (narrow-gap system), it costs less energy (more energy) to excite  $N$  bosons from  $E_0$  to  $E_1$  than to excite one boson from  $E_1$  to  $E_2$ , i.e., across the energy gap. We note that a bosonic system initially in the wide-gap category can be gradually driven towards the narrow-gap region if  $N$  is increased while the potential is kept fixed. During such a transition, one would expect observable concomitant

Reprint requests to Dr. K. L. Liu; Fax: (852) 2603 5204, E-mail: klliu@phy.cuhk.edu.hk

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changes in the thermodynamic quantities of the system, such as the heat capacity.

This paper is organized as follows. In Sect. 2 we first consider the simpler wide-gap system and analyze some of its generic thermodynamic behavior at low temperatures. The numerical results for the more complex case of an ideal Bose gas in a three-dimensional (3D) superposition of symmetric double-well potentials at finite temperatures are presented and discussed in Section 3. Our conclusions are given in Section 4.

## 2. Wide-gap System at Low Temperatures

Since the wide-gap condition  $G > N\Delta$  is realizable, it is useful to examine the thermodynamics of a bosonic wide-gap system at low temperatures, as described by the grand canonical ensemble [12, 15], with the thermal energy  $k_B T < G$ , where  $k_B$  is the Boltzmann constant, and  $T$  is the absolute temperature.

So far as the determination of the chemical potential  $\mu$  at such low temperatures is concerned, it is sufficient to only take into account the populations  $N_0$  and  $N_1$  in the ground state and the first excited state respectively; this is to be referred to as the single-doublet approximation for  $\mu$ . However, in terms of energy considerations, the wide-gap system has a somewhat unusual feature: even though the particles in the second excited state have a negligibly small population  $N_2$  at low  $T$ , their contribution to the average total energy  $U$  of the system may not be insignificant. In other words, one can have  $N_2 \ll N_1$ , and yet  $N_2 G \approx N_1 \Delta$ . We are thus led to introduce a threshold temperature  $T_E$  below which the contribution associated with  $N_2$  to  $U$  can be safely ignored:

$$G \times \exp(-G/k_B T_E) = \Delta \quad (1)$$

which yields

$$k_B T_E = [G/\ln(G/\Delta)] \ll G \quad (2)$$

In Eq. (1) we use the Boltzmann factor as an estimate for  $N_2$  and set the energy contribution equal to the smallest single-particle excitation energy  $\Delta$ . We note that  $T_E$  is solely determined by the single-particle potential  $V$ . On the other hand, as shown below, our analysis brings forward several useful  $N$ -dependent characteristic temperatures:  $T_j = N^j \Delta/k_B$  with  $j = \frac{1}{3}, \frac{1}{2}, 1$ . For the values of  $N$  of interest ( $10^3 \leq N \leq 10^7$ ), we have  $T_{1/3} \ll T_{1/2} \ll T_1$ . Obviously, if  $N$  is allowed to vary while  $V$  is fixed, one can change the magnitude of  $T_j$  relative to  $T_E$ ; this has important effects on the thermal variation of the heat capacity  $C(T)$ .

For simplicity, we assume that both  $E_1$  and  $E_2$  are non-degenerate; the extension to the more general cases will be mentioned at the end of this section. In the single-doublet approximation, the chemical potential is determined by the relation

$$N = N_0 + N_1 = \frac{1}{(\xi - 1)} + \frac{1}{(\eta \xi - 1)} \quad (3)$$

where  $\xi = \exp[\beta(E_0 - \mu)]$ ,  $\eta = \exp(\beta\Delta)$ , and  $\beta = (k_B T)^{-1}$ . The appropriate solution of Eq. (3) yields

$$\xi = \frac{1}{2\eta} \left\{ \left( 1 + \frac{1}{N} \right) (\eta + 1) + \left[ \left( 1 + \frac{2}{N} \right) (\eta - 1)^2 + \frac{1}{N^2} (\eta + 1)^2 \right]^{1/2} \right\} \quad (4)$$

which satisfies  $\xi \rightarrow (1 + N^{-1})$  as  $T \rightarrow 0$ . It is useful to note that in the whole temperature range  $0 \leq k_B T < G$ ,  $\xi$  is a very slowly varying function of  $T$  for large  $N$ . More explicitly, analysis of Eq. (4) shows that  $\xi(T) = [1 + N^{-1} + O(N^{-3/2})]$  for  $0 < T \leq O(T_{1/2})$ ,  $\xi(T_1) = [1 + 1.62N^{-1} + O(N^{-2})]$ , and  $\xi \approx (1 + 2N^{-1})$  if  $T_1 \ll T < (G/k_B)$ .

With  $\xi$  so determined, we now proceed to study  $U$  and  $C$ , and start with such a value of  $N$  that  $T_E \gg T_1$ . For the potential  $V(8; x)$ , this assumption restricts  $N \ll 3 \times 10^4$  while for  $V(10; x)$ ,  $N \ll 7 \times 10^6$ . When the above condition is satisfied, the heat capacity will exhibit several generic features, as shown below.

When  $0 < T \leq O(T_{1/2})$ , we can use the approximation  $\xi \approx (1 + N^{-1})$  to calculate  $N_1$ . The average total energy is then given by

$$U = N E_0 + N_1 \Delta \approx N E_0 + \frac{\Delta}{(1 + N^{-1})(\eta - 1 + N^{-1})} \quad (5)$$

Consequently, the heat capacity at constant  $N$  is found to be

$$C_1 = \frac{k_B}{(1 + N^{-1})} \cdot \frac{(\beta \Delta)^2 \eta}{(\eta - 1 + N^{-1})^2} \quad (6)$$

where the notation  $C_1$  emphasizes that only the lowest energy-doublet has been taken into account. As expected,  $C_1$  is exponentially small at extremely low temperatures. However, when  $T$  is raised from the absolute zero,  $C_1$  shows an initial sharp rise. Analysis of Eq. (6) reveals that  $C_1$  attains its maximum at a characteristic temperature  $T^*$  which is below  $T_{1/2}$ :

$$T^* = \left[ \frac{1}{J} + \frac{3}{5J^2 N^{2/3}} + O\left(\frac{1}{N^{4/3}}\right) \right] \times T_{1/3} \quad (7)$$

where  $J=(12)^{1/3}$  is a numerical constant. At this temperature,  $C_1$  is close to  $1 k_B$ :

$$\frac{C_1(T^*)}{k_B} = 1 - \frac{J^2}{4N^{2/3}} + O\left(\frac{1}{N^{4/3}}\right) \quad (8)$$

and only a negligibly small fraction of the bosons occupies the first excited state:

$$\frac{N_1(T^*)}{N} = \frac{1}{JN^{2/3}} - \frac{1}{2N} + O\left(\frac{1}{N^{4/3}}\right). \quad (9)$$

Above  $T^*$ ,  $N_1$  grows with increasing  $T$ . When  $T=O(T_{1/2})$ , we find that

$$N_1(T) = \left(\frac{k_B T}{\Delta}\right) \left[ 1 - \frac{1}{2} \beta \Delta - \frac{1}{N \beta \Delta} + \frac{1}{12} (\beta \Delta)^2 + \frac{1}{(N \beta \Delta)^2} + O\left(\frac{1}{N^{3/2}}\right) \right] \quad (10)$$

which increases approximately linearly with  $T$ . At the same time,  $C_1$  decreases slowly with increasing  $T$ :

$$\frac{C_1(T)}{k_B} = 1 - \frac{2}{N \beta \Delta} - \frac{1}{12} (\beta \Delta)^2 + \frac{3}{(N \beta \Delta)^2} + O\left(\frac{1}{N^{3/2}}\right). \quad (11)$$

The deviation of  $C_1(T)$  from  $1 k_B$  varies approximately linearly with  $T$ , the rate of the linear-drop being dependent on  $N^{-1}$ . Nevertheless, we observe that the heat capacity is essentially a universal constant  $C \approx 1 k_B$  in the temperature interval  $T^* \leq T \leq T_{1/2}$  for large  $N$ .

$N_1$  reaches the value  $0.38 N$  at  $T_1$ . When  $T_1 \ll T < T_E$ , we find that

$$N_1(T) = \left(\frac{N}{2}\right) \left(1 - \frac{1}{2} N \beta \Delta\right) \quad (12)$$

which shows that approximately half of the bosons has been thermally excited out of the ground state at this temperature. Concomitantly, the heat capacity becomes small compared with  $1 k_B$

$$\frac{C_1(T)}{k_B} \approx \left(\frac{1}{2}\right)^2 (N \beta \Delta)^2 \quad (13)$$

and it exhibits a rapid inverse-square drop with increasing  $T$ :  $C_1 \sim T^{-2}$ .

Upon further heating of the system so that  $T_E < T < (G/k_B)$ , the approximation of  $C(T)$  by  $C_1(T)$  is no longer valid. We must now include the contribution to  $U$  due to particles thermally excited to the second

energy doublet ( $E_2, E_3$ ). Consequently, an additional contribution  $C_2(T)$  is introduced to  $C(T)$ :  $C(T) = C_1(T) + C_2(T)$  with

$$C_2(T) = \sum_{j=2}^3 \frac{k_B (\beta E_{j0})^2 \eta_j}{\xi(\eta_j - \xi^{-1})^2}, \quad (14)$$

where  $E_{j0} = E_j - E_0$ ,  $\eta_j = \exp(\beta E_{j0})$ , and the approximation  $\xi = 1 + 2N^{-1}$  can be used. Within this temperature range, one can show that  $C_2(T)$  is a monotonically increasing function of  $T$ . Therefore, subsequently to the inverse-square drop described by Eq. (13), the heat capacity rises with increasing  $T$  in the temperature interval  $T_E < T < (G/k_B)$ .

The above discussion concentrates on systems with  $T_E \gg T_1$ . In order to confirm the validity of the analysis, we present in Fig. 1 the numerical results for the potential  $V(8; x)$ . The numerical calculations use the general formulae

$$N = \sum_{j=0}^{\infty} \{ \exp[\beta(E_j - \mu)] - 1 \}^{-1} \equiv \sum_{j=0}^{\infty} n_B(E_j)$$

and  $U = \sum_{j=0}^{\infty} E_j n_B(E_j)$

to determine  $\mu$  and the average total energy  $U$  at a general temperature  $T$ . The heat capacity  $C(T) = (\partial U / \partial T)_N$  is then obtained by numerical differentiation. The eigenenergies  $\{E_j\}$  and the normalized eigenfunctions  $\{\psi_j(x)\}$  are calculated by the state-dependent diagonalization (SDD) method of [16] which is especially efficient for the high excited states. We find that the numerical results of the eigenvalues  $E_n$  with  $n \geq 100$  can be accurately represented by the following formula which is suggested by the WKB approximation:

$$E_n = 1.3765 \hbar \omega \times (s^4 - 3.1168 s^2 - 2.0768), \quad (15)$$

where  $s = (n + 0.5)^{1/3}$ .

For  $V(8; x)$ , we have  $k_B T_E \approx 0.4 \hbar \omega$  and  $G \approx 5 \hbar \omega$ . According to the above analysis, we should have the following results when  $N=2000$ :  $C(T^*) \approx 1 k_B$  at  $k_B T^* = 9 \times 10^{-5} \hbar \omega$ ;  $C(T)$  shows a very weak decrease in the temperature range  $9 \times 10^{-5} \hbar \omega < k_B T < 7 \times 10^{-4} \hbar \omega$ , and it then shows a  $T^{-2}$ -drop when  $0.03 \hbar \omega \ll k_B T < 0.4 \hbar \omega$ . For  $N=1000$ , the corresponding results are:  $k_B T^* = 7 \times 10^{-5} \hbar \omega$ , the linear-drop region of  $C(T)$  shifts to  $7 \times 10^{-5} \hbar \omega < k_B T < 5 \times 10^{-4} \hbar \omega$ , and the  $T^{-2}$ -drop occurs when  $0.02 \hbar \omega \ll k_B T < 0.4 \hbar \omega$ . Besides,  $C(T)$  should, in both cases, rise with increasing  $T$  in the temperature range  $0.4 \hbar \omega < k_B T < 5 \hbar \omega$ . As can be seen from Fig. 1 b,

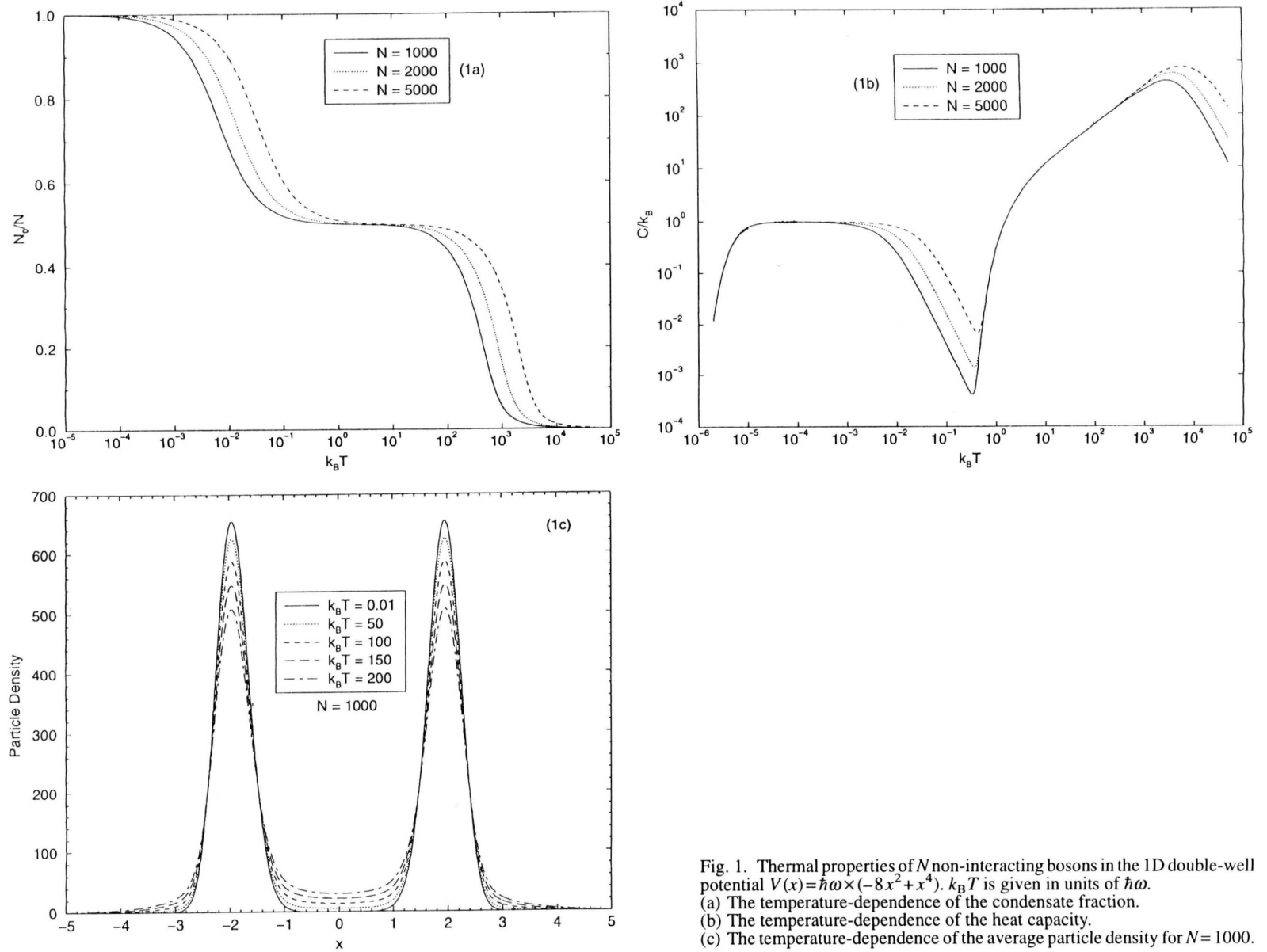


Fig. 1. Thermal properties of  $N$  non-interacting bosons in the 1D double-well potential  $V(x) = \hbar\omega \times (-8x^2 + x^4)$ .  $k_B T$  is given in units of  $\hbar\omega$ .  
(a) The temperature-dependence of the condensate fraction.  
(b) The temperature-dependence of the heat capacity.  
(c) The temperature-dependence of the average particle density for  $N = 1000$ .

the predictions of the analysis are in excellent agreement with the numerical results.

In Fig. 1c, we plot the average particle density  $D(x) = \sum_{j=0}^{\infty} n_B(E_j) |\psi_j(x)|^2$  for  $N=1000$  at various temperatures. When the system is in its ground state, the bosons are mainly localized in the vicinities of the potential minima, and hence  $D(x)$  shows two symmetrical distinct peaks at  $x=\pm 2$ . However, as  $T$  increases, some bosons acquire sufficient thermal energy to overcome the potential barrier at  $x=0$ , and we witness a gradual delocalization of the particle density from the bottoms of the potential wells.

When the condition  $T_E \gg T_1$  is violated, the aforementioned low-temperature features of  $C(T)$  will be modified. In general, in the entire temperature range  $0 < k_B T < G$ , it is sufficient to take  $C(T) = C_1(T) + C_2(T)$ , with the threshold temperature  $T_E$  providing a gauge for the relative importance of  $C_2$ . If  $N$  is so large that  $T_{1/2} \ll T_E \leq T_1$ , the simple  $T^{-2}$ -drop region, predicted by Eq. (13), will not be seen in  $C(T)$  owing to the serious intervention of  $C_2(T)$ . In this case, however,  $C(T)$  still possesses the weak linear-drop region described by Eq. (11). [For the potential  $V(8; x)$ , this happens when  $3 \times 10^4 \leq N \ll 6 \times 10^8$ .] If  $N$  is further increased so that  $T^* \ll T_E \leq T_{1/2}$ , even the linear-drop region will not be discernible in  $C(T)$ , although the local maximum of  $C$  at  $T^*$  still exists. [For  $V(8; x)$ , this takes place when  $6 \times 10^8 \leq N \ll 2 \times 10^{14}$  in which case the system belongs to the narrow-gap category.] Finally if  $T_E \ll T^*$ ,  $C(T)$  will not have a Schottky-type peak at low temperatures.

The analysis of  $C_1(T)$  can be extended to the case when  $E_1$  is  $d_1$ -fold degenerate and  $E_2$  is  $d_2$ -fold degenerate. The threshold temperature is now defined by  $k_B T'_E = [G/\ln(d_2 G/\Delta)]$  which is below the previous  $T_E$ . It can be shown that the maximum of  $C_1$  still occurs at the characteristic temperature  $T^*$  as given in Eq. (7), but the value of the maximum is enhanced by a factor of  $d_1$ :  $C_1(T^*) \approx d_1 \times k_B$ . In addition, the numerical prefactor  $(\frac{1}{2})^2$  in Eq. (13) should now be replaced by the even smaller factor  $d_1/(d_1+1)^2$ .

### 3. Bosons in the Field of Superimposed Double-well Potentials

To further investigate the effects of double-well potentials, we now turn to study bosons trapped in a confining potential  $V(\mathbf{r})$  which is generated by superimposing three 1D double-well potentials. As a specific exam-

ple, we take

$$V(\mathbf{r}) = \hbar\omega \times \sum_{i=1}^3 (-A_i x_i^2 + x_i^4) = \sum_{i=1}^3 V_i(x_i) \quad (16)$$

where  $A_i$  are positive constants, and  $\{x_i\}$  are dimensionless co-ordinates. The eigenenergies of  $V(\mathbf{r})$  are simply formed by the sum of the eigenenergies of the three constituent potentials. In order to study the thermodynamic properties for a wide range of  $N$  and  $T$ , we have calculated a large number of eigenvalues for two 1D double-well potentials, namely,  $(-8x^2 + x^4)$  and  $(-10x^2 + x^4)$ , by the SDD method [16].

As the first example, we consider the potential  $V_a(\mathbf{r})$  with  $A_i=8$ , which corresponds to the superposition of three identical 1D double-well potentials. The results for the thermodynamic properties of the trapped bosons are shown in Fig. 2, where we use  $T_0 \equiv (\hbar\omega/k_B) [N/\zeta(3)]^{1/3}$ , the BEC temperature for bosons in an isotropic 3D harmonic trap [7], as a convenient unit of temperature. As shown in Fig. 2a, for a system with  $N = O(10^3)$ , the condensate fraction ( $N_0/N$ ) starts to deviate appreciably from unity at  $T \approx 10^{-4} T_0$ , and then rapidly falls to the value of approximately one-eighth at  $T \approx 10^{-3} T_0$ , which implies the occurrence of considerable particle excitations from the ground state even at this low temperature. This can be understood based on the eigenenergies listed in Table 1. It can be easily shown that the first 8 eigenstates of the composite potential  $V_a$  have eigenenergies very close to one another:  $E_1$  and  $E_2$  are 3-fold degenerate and the energy difference between adjacent energy levels is  $\Delta E = 1.6 \times 10^{-5} \hbar\omega$ . On the other hand, there is a much larger energy gap  $G_9 = 5.2 \hbar\omega$  between this low-energy group and the 9th eigenstate. Thus, at the temperature  $k_B T = N \Delta E = 1.7 \times 10^{-5} N^{2/3} k_B T_0 = O(10^{-2} \hbar\omega)$ , the 9th and the higher eigenstates are practically unoccupied, while the lowest 8 eigenstates are approximately equally populated, yielding  $(N_0/N) \approx \frac{1}{8}$ . This situation persists until  $k_B T \gg G_9$ . Moreover, the total heat capacity  $C_V$  of the system exhibits some interesting microstructure within the temperature range  $10^{-7} T_0 < T < 10^{-3} T_0$ , as shown in Figure 2b. There exists a small peak at  $T \approx 10^{-5} T_0$ ; but  $C_V$  falls rapidly when  $10^{-3} T_0 \leq T \leq 10^{-2} T_0$ . Such behavior of  $C_V$  can also be qualitatively understood in terms of the structure of the eigenvalue spectrum of the system. Consider temperatures in the range  $3 \Delta E \ll k_B T \ll G_9$ . In the first estimate for  $C_V$ , we may replace the 7 lowest excited states by one effective 7-fold degenerate energy level with an energy  $\bar{E}_1$  equal to their average energy. This approximation leads to an effective tunneling energy splitting  $\bar{\Delta} = 2.7 \times 10^{-5} \hbar\omega$ . Then, according to our dis-



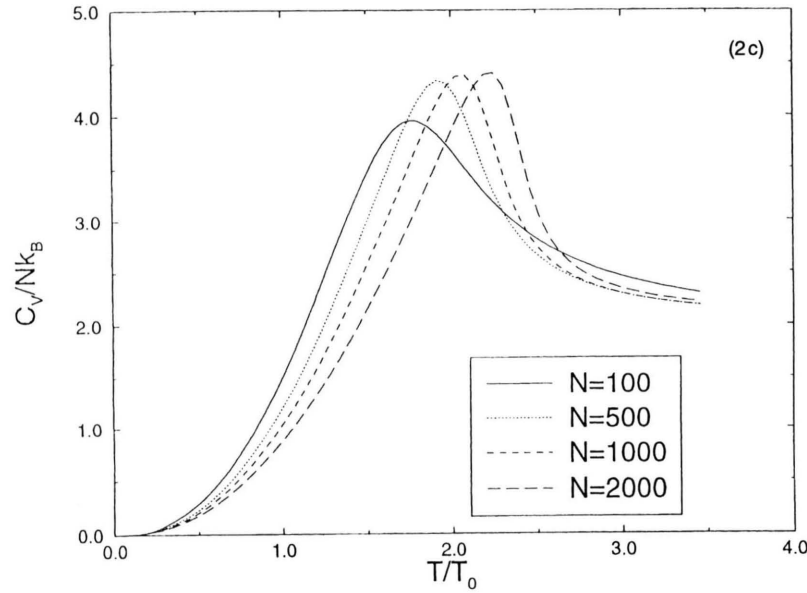
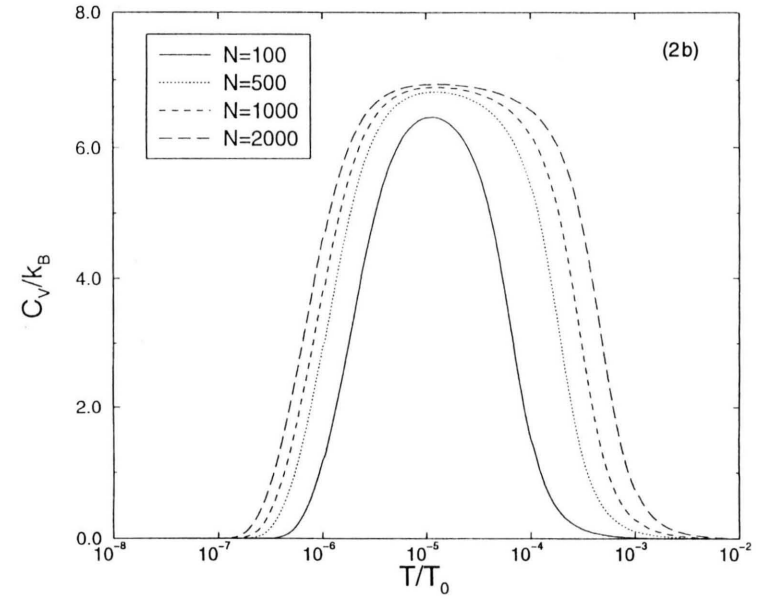
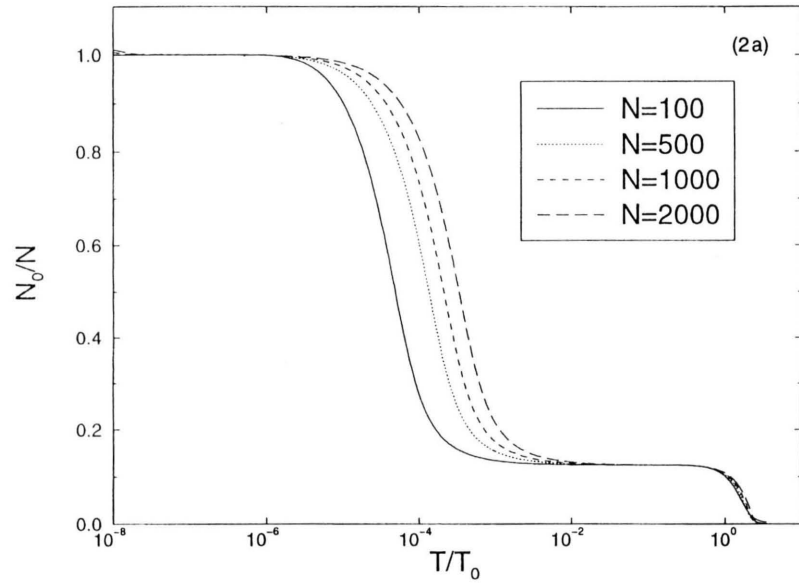


Fig. 2. Thermal properties of  $N$  non-interacting bosons in the field of the 3D confining potential  $V_a(\mathbf{r})$ . For each value of  $N$ , the temperature is measured in units of  $T_0 = (\hbar\omega/k_B) [N/\zeta(3)]^{1/3}$ . (a) The temperature-dependence of the condensate fraction. (b) The microstructure of the heat capacity at low temperatures. (c) The thermal variation of the heat capacity per particle. The microstructure of Fig. 2b is not discernible on the scale of this graph.

Table 1. The first few eigenenergies of the 1D double-well potential  $V(x) = -Ax^2 + x^4$ : (a)  $A=8$ , (b)  $A=10$ .

$n$	$E_n(a)$	$E_n(b)$
0	-13.23759407	-21.88965828
1	-13.23757818	-21.88965823
2	-8.01109597	-15.89346574
3	-8.00899818	-15.89345480
4	-3.40382817	-10.28612581

cussion for a wide-gap system with a degenerate  $E_1$ , we shall anticipate the appearance of a Schottky-type peak with the value  $C_V(T^*) = 7k_B$ , followed by the  $T^{-2}$ -drop region as mentioned before. Indeed, estimates of the characteristic temperatures based on the parameters  $\bar{A}$  and  $G_0$  are found to be in satisfactory agreement with the numerical results. For example, for  $N=2000$ , our estimates are  $T^* = 1.5 \times 10^{-4} (\hbar\omega/k_B) = 1.3 \times 10^{-5} T_0$ ,  $T_{1/2} = 1.0 \times 10^{-4} T_0$ ,  $T_1 = 4.5 \times 10^{-3} T_0$ , and  $T_E = 3.6 \times 10^{-2} T_0$ . The estimates are less accurate for  $N=100$  since the corresponding  $T^*$  is only slightly larger than  $3\Delta E$ .

Finally, we turn to the case when the three 1D double-well potentials are not all identical. As a specific example, we take the potential  $V_b(\mathbf{r})$  with  $(A_1, A_2, A_3) = (10, 10, 8)$ .  $V_b$  represents a superposition of two identical 1D double-well potentials with another shallower double well potential. The numerical results of this new confined system are shown in Figure 3. Again we see that the condensate fraction drops rapidly from unity to one-eighth as  $T$  is raised from the absolute zero to  $T \approx 10^{-2} T_0$  for the values of  $N$  studied. However, instead of a ‘single-step’ process as in the previous case, the depletion of  $(N_0/N)$  towards  $\frac{1}{8}$  actually takes place in ‘two steps’ for the present system, as one may infer from the curves shown in Figure 3a. This interesting process arises from the fact that the eigenenergy spectrum of the 1D double-well potential in the  $x_3$  direction is no longer identical to those of the other two double-well potentials. Consequently, the lowest eight eigenstates are now split into two subgroups, each one composed of four nearly degenerate energy levels, as listed in Table 2. Thus, as  $T$  increases from the absolute zero, one expects that  $(N_0/N)$  first falls to the value  $\frac{1}{4}$  at a temperature  $T \approx N \times 10^{-7} (\hbar\omega/k_B) = 1.1 \times 10^{-7} N^{2/3} T_0$  when the lowest four nearly degenerate energy levels are almost equally populated. With a slower pace the condensate fraction continues to diminish with increasing  $T$ , reaching the value of  $\frac{1}{8}$  at  $T \approx N \times 1.6 \times 10^{-5} (\hbar\omega/k_B) = 1.7 \times 10^{-5} N^{2/3} T_0$ . At this point, all the eight lowest eigenstates are approximately evenly occupied by the bosons with the higher

energy levels being almost unfilled. Furthermore, the low-temperature heat capacity displays a two-peak microstructure as well. When  $k_B T \leq 10^{-7} \hbar\omega$ , the heat capacity is dominated by the contribution from the first group of four nearly degenerate eigenstates: they are responsible for the approximate  $3k_B$ -peak observed in  $C_V(T)$ . As can be seen from Fig. 3b, the  $3k_B$ -peak becomes less pronounced when the number of the trapped bosons increases. Such a trend is in accord with the discussion of Section 2. It is also of interest to note the development of the second peak of  $C_V(T)$  as  $N$  increases. We observe that the second peak gradually approaches  $7k_B$  when  $N$  is increased from  $5 \times 10^3$  to  $5 \times 10^4$ , and that this peak appears at a temperature  $T_2^* \sim 10^{-6} T_0$ . We may again estimate  $T_2^*$  by approximating the seven lowest excited states by a 7-fold degenerate energy level: such an approximation procedure is meaningful when  $k_B T \gg 10^{-5} \hbar\omega$ . For  $N = 5 \times 10^4$ , we obtain the estimate  $T_2^* = 4.2 \times 10^{-6} T_0$  which agrees fairly well with the numerical result.

Besides the microstructures found at low temperatures, the heat capacity also displays a conspicuous high-temperature maximum, whose magnitude is of the order of  $Nk_B$ , at a characteristic temperature  $T_h$ , as shown in Figs. 2c and 3c. In the case of  $V_b$ , the numerical data for  $2000 \leq N \leq 50,000$  indicate that the high-temperature maximum of  $C$  appears in the immediate vicinity of the on-set of the BEC, with  $T_h$  only slightly below the BEC temperature  $T_c$ . Moreover, in this range of  $N$ , both  $T_h$  and  $T_c$  are found to be approximately proportional to  $N^{0.45}$ . This  $N$ -dependence is quite close to the scaling law  $T_c \sim N^{4/9}$  predicted by the semiclassical theory for bosons in the quartic confining potential

$$V(\mathbf{r}) = \sum_{i=1}^3 a_i x_i^4 \quad [17].$$

We also note that for a given  $N$ , the BEC temperature corresponding to the 3D potential  $V_a(\mathbf{r})$  is much lower than that for the 1D counterpart  $V(8; x)$ . An analogous result was previously obtained for the harmonic traps [8].

Table 2. The first eight energy levels of the three-dimensional confining potential  $\tilde{V}_b(\mathbf{r})$ . The ground state energy is taken as the energy origin. The eigenenergies are given in units of  $\hbar\omega$ .

State	Eigenenergy	Degeneracy
Ground state	0.0	1
1 <sup>st</sup> excited state	$5.0 \times 10^{-8}$	2
2 <sup>nd</sup> excited state	$1.0 \times 10^{-7}$	1
3 <sup>rd</sup> excited state	$1.590 \times 10^{-5}$	1
4 <sup>th</sup> excited state	$1.595 \times 10^{-5}$	2
5 <sup>th</sup> excited state	$1.600 \times 10^{-5}$	1

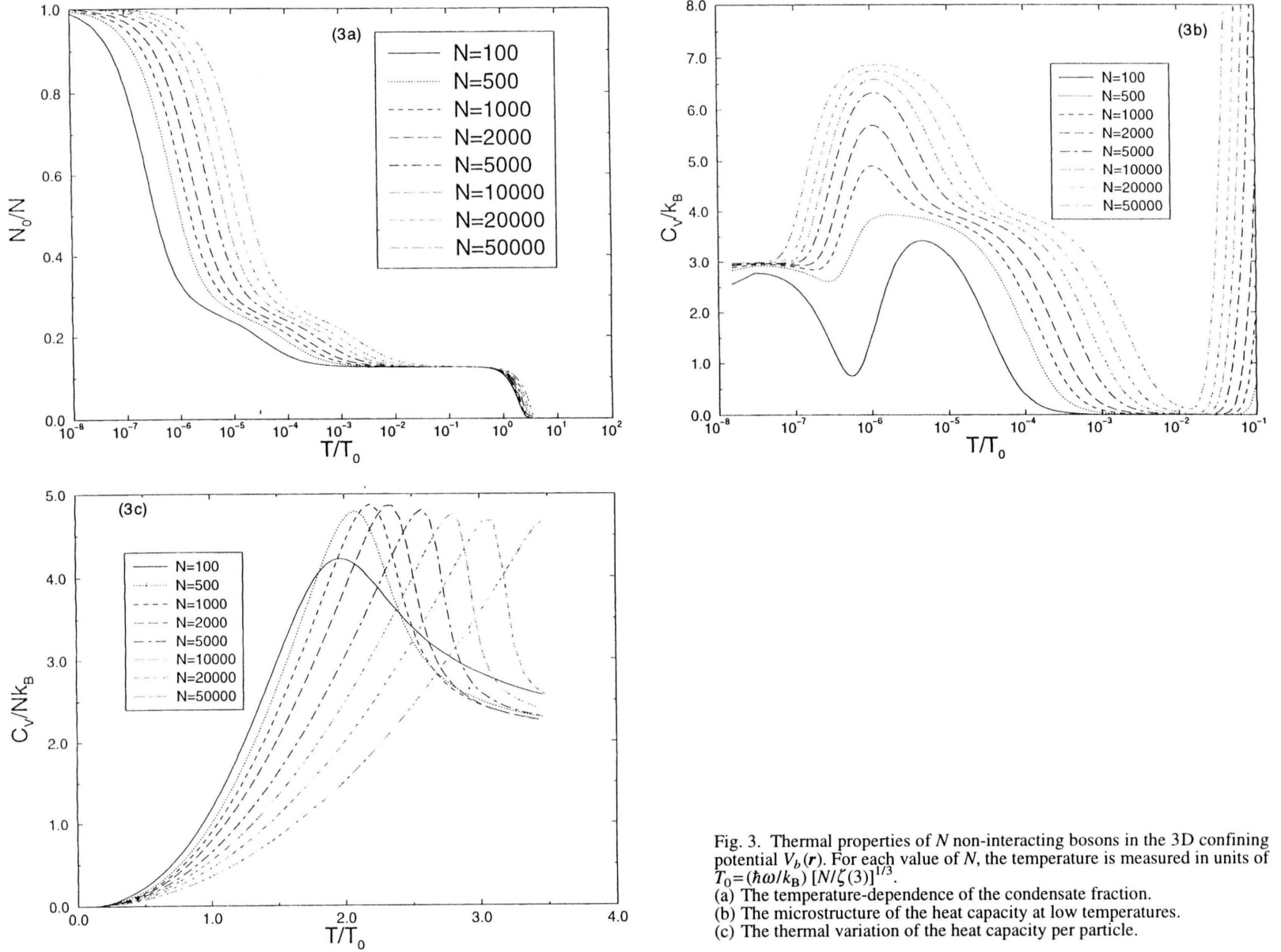


Fig. 3. Thermal properties of  $N$  non-interacting bosons in the 3D confining potential  $V_b(r)$ . For each value of  $N$ , the temperature is measured in units of  $T_0 = (\hbar\omega/k_B) [N/\zeta(3)]^{1/3}$ .  
(a) The temperature-dependence of the condensate fraction.  
(b) The microstructure of the heat capacity at low temperatures.  
(c) The thermal variation of the heat capacity per particle.



#### 4. Conclusion

Bosons in the field of a double-well potential are of considerable physical interest, especially from the point of view of observing coherent quantum tunneling of the Bose condensate [18, 19]. In this work, we concentrate on the thermodynamic aspects of systems with deep double-well potentials, and have found some generic results for the condensate fraction as well as the heat capacity  $C$ .

For potentials of the  $V_a$ -type or the  $V_b$ -type, the thermal variation of the condensate fraction shows a marked one-eighth plateau below  $T_c$ . In addition, for potentials of the  $V_a$ -type, the low temperature heat capacity displays a Schottky-type peak with a magnitude of approximately  $7k_B$  at a characteristic temperature  $T^* \sim N^{1/3}$ . For potentials of the  $V_b$ -type, a more complicated microstructure with two peaks can be observed in the thermal variations of  $C$  at low  $T$ .

We have shown that the number of bosons  $N$  has an important effect on the shape of  $C(T)$  at low temperatures. For example, as  $N$  increases, the aforementioned

two-peak microstructure of  $C(T)$  will evolve to form a single peak with the magnitude  $C \approx 7k_B$ .

We emphasize that all these low-temperature features originate from the generic structure of the eigenenergy spectrum of the low-lying excited states; they are not specific to the quartic double-well potentials. The essential ingredient is the existence of groups of low-lying excited states for which the intra-group energy-level spacings are far smaller than the inter-group energy differences. On the other hand, the BEC temperature  $T_c$  depends on the form of the potential used [17]. For the 3D superpositions of quartic double-well potentials studied in this work, we find that  $T_c$  approximately scales with  $N^{0.45}$ . Finally, it will be of interest to study how the inclusion of inter-particle interactions will affect the results presented here.

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