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# Heat capacity of trapped bosons in a combined harmonic-lattice potential

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## Abstract

In this paper, the heat capacity per particle  $C(T)/Nk_B$  of the trapped bosons in a combined harmonic-lattice potential is calculated within the semiclassical approximation. The main effects which can alter the ideal gas are included simultaneously in the present approach. The calculated results show that the heat capacity has a significant dependence on the lattice depth and temperature. Classical results are recovered at sufficiently high temperature, and that it reproduces the Dulong-Petit law type. Moreover, the behavior of the heat capacity in a deep lattice can be used as an indicator for the quantum phase transition superfluid-Mott insulator. It decreases as the system gets closer to the Mott transition. The calculated results provide a solid theoretical foundation of the current experiments.

**Key Words:** Thermodynamical properties for BEC in optical lattice; semiclassical theories and applications

## 1. Introduction

Ultracold boson atoms stored in a combined harmonic-lattice potential (lattice bosons) display a great variety of quantum phenomena, similar to those found in certain solid-state systems [1]. However, by using external fields the atoms can be brought to new experimental regimes and allow one to explore novel phenomena, such as superfluid (SF)-Mott insulator (MI) quantum phase transition [2]. In this context, calculation of the thermodynamic quantities, such as the heat capacity per a particle at constant volume  $C_V(T)/Nk_B$  is of considerable interest. Its behavior can be used as an indicator for the possible quantum SF-MI phase transitions [3].

In the present paper an analytical semiclassical approximation, which is the density of states (DOS) approach, for calculating  $C_V(T)/Nk_B$  is given. This approach is based on using a piecewise DOS to convert the sum over quantum state for the thermodynamical quantities into an ordinary integral directly [4]. The parametrized DOS allows the inclusion of the main effects which can alter the ideal gas, such as the finite size effect directly [5] and the effect of interatomic interaction indirectly [6]. The obtained formula for the thermodynamic quantities as a function of temperature is given in terms of two scaling parameters. The first

parameter parametrizes the effect of anisotropic hopping in the optical lattice. While the second parameter accounts the finite size, interatomic interaction and deepness of the lattice potential effects. The calculated results show that the heat capacity is accompanied by a peak in the higher temperature range (below the Bose Einstein condensation temperature) for both anisotropic or isotropic harmonic potential, providing that there is highly anisotropic hopping in the optical lattice.

Remainder of this paper is organized as follows. A simple model for the theoretical framework of BEC in a combined potential is given in section two. The heat capacity is calculated in section three. The last section outlines the discussion and conclusions.

## 2. Theoretical model

The combined potential is set up by accompanying an optical potential with a magnetic confining potential [7]. The optical (lattice) potential,  $V_{\text{lat}}(\mathbf{r}) = [V_x \sin^2(kx) + V_y \sin^2(ky) + V_z \sin^2(kz)]$ , is created by combining multiple laser beams with suitable alignment and polarization. While the magnetic (harmonic) potential,  $V_{\text{har}}(\mathbf{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$ , is arising from an external magnetic potential with frequencies  $\{\omega_x, \omega_y, \omega_z\}$ . The potential seen by the atoms is typically modeled in the form [8]

$$V_{\text{com}}(\mathbf{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \quad (1)$$

$$+ E_R [s_x \sin^2(kx) + s_y \sin^2(ky) + s_z \sin^2(kz)], \quad (2)$$

where  $s_{x,y,z} = V_{x,y,z}/E_R$  is a dimensionless parameter which denotes the lattice depth  $V_{x,y,z}$  in units of the recoil energy  $E_R$ . The recoil energy,  $E_R = \frac{\hbar^2 k^2}{2m}$   $\{\equiv \hbar\omega_R\}$ , is defined as the recoil energy that one atom acquires as it absorbs one lattice photon, and  $k = 2\pi/\lambda$  is the lattice wave number, where  $\lambda$  is the laser wavelength.

In order to use Bose-Einstein statistics in calculating  $C(T)/Nk_B$  for this system, the single particle energy levels are needed. For potential (2), it is impossible to find an exact analytical expression for the energy of these levels. An approximate expression can be readily obtained if the trapped atoms are considered to be harmonically trapped in the ground state of the optical lattice. In this case, the single particle energy levels can be approximated by a modified harmonical oscillator energy levels.

However, for sufficiently deep optical lattice the confinement of an individual lattice site can be approximated by a corresponding harmonic potential with  $\omega_{\text{lat},x,y,z} = [(2V_{x,y,z}k^2)/m]^{1/2}$  plus a quartic term which can be treated perturbatively via the normal ladder operators. Under this approximation the single particle energy level is given by [9, 10],

$$E_n = n_x \hbar \omega'_x + n_y \hbar \omega'_y + n_z \hbar \omega'_z + E_0, \quad (3)$$

where  $E_0 = \frac{3}{2} \hbar \bar{\omega}$  with  $\bar{\omega} = \frac{1}{3}(\omega'_x + \omega'_y + \omega'_z)$  is the mean of the combined frequencies, and  $\omega'_{x,y,z}$  are given by

$$\begin{aligned} \omega'_x &= \omega_x [\sqrt{1 + 4s_x t_x^2} - 0.5t_x], \\ \omega'_y &= \omega_y [\sqrt{1 + 4s_y t_y^2} - 0.5t_y], \\ \omega'_z &= \omega_z [\sqrt{1 + 4s_z t_z^2} - 0.5t_z], \end{aligned} \quad (4)$$

where  $t_{x,y,z} = \frac{\omega_R}{\omega_{x,y,z}}$  gives the ratio between recoil frequency and geometrical average of the harmonic frequencies.

BEC is described within the grand canonical ensemble. Its relevant thermodynamic quantities can be calculated from the partial derivative of the corresponding thermodynamical potential  $q$  of the physical system. For a trapped Boson in a combined potential the thermodynamical potential  $q$  is given by [11, 12],

$$q = - \sum_n g_n \ln (1 - ze^{-\beta E_n}), \quad (5)$$

where  $\beta = (1/k_B T)$  and  $k_B$  is the Boltzmann constant,  $z = e^{\beta(\mu_k - E_0)}$  is the fugacity and  $g_n = (\frac{1}{2}n^2 + \frac{3}{2}n + 1)$  is the degeneracy of the energy levels of the harmonic potential. It is convenient to expand the logarithm to express the grand potential as a sum over Bose-Einstein distribution and using the semiclassical approximation (summation over  $n$  in equation (5) is converted into an integral weighted by a DOS  $\rho(\epsilon)$ ):

$$\begin{aligned} q &= q_0 + \sum_{n=1}^{\infty} \frac{g_n z e^{-\beta E_n}}{1 - z e^{-\beta E_n}} \\ &= q_0 + \sum_{j=1}^{\infty} \frac{z^j}{j} \int_0^{\infty} \rho(\epsilon) e^{-j\beta\epsilon} d\epsilon, \end{aligned} \quad (6)$$

The analytic DOS, which is relatively accurate for the lattice depths and harmonic confinements used in experiments, is calculated for the spectrum (3) in [8, 9] as

$$\rho(\epsilon) = \frac{1}{\gamma^3} \left[ \frac{1}{2} \frac{\epsilon^2}{(\hbar\Omega)^3} + \frac{\epsilon}{(\hbar\Omega)^2} \left[ \frac{3}{2} \frac{\bar{\omega}}{\Omega} + \frac{2}{3} \frac{\mu_k}{\hbar\bar{\omega}} \gamma \right] \right], \quad (7)$$

where  $\Omega = [\omega_x \omega_y \omega_z]^{1/3}$  is the geometrical average of the harmonic frequencies, and  $\mu_k$  is the chemical potential. The parameter  $\gamma$  is given by

$$\gamma = \left[ [\sqrt{1 + 4s_x t_x^2} - 0.5t_x] [\sqrt{1 + 4s_y t_y^2} - 0.5t_y] [\sqrt{1 + 4s_z t_z^2} - 0.5t_z] \right]^{1/3} \quad (8)$$

The parameter  $\gamma$  parametrizes the effects of anisotropic hopping through  $t$ 's and the deepness of the optical lattice potential through  $s$ 's. It is clear that in the absence of the optical potential,  $\gamma = 1$ . For deep lattice and small relative frequency,  $\gamma \gg 1$ .

Substituting from equation (7) in (6), one has

$$q = q_0 + \gamma^{-3} \left[ \left( \frac{K_B T}{\hbar\Omega} \right)^3 g_4(z) + \left( \frac{K_B T}{\hbar\Omega} \right)^2 g_3(z) \left\{ \frac{3}{2} \frac{\bar{\omega}}{\Omega} + \frac{2}{3} \frac{\mu_k}{\hbar\bar{\omega}} \gamma \right\} \right], \quad (9)$$

where  $q_0 = -\ln(1 - z)$ , and  $g_k(z) = \sum_{j=1}^{\infty} (z^j / j^k)$  is the usual Bose function. The intuitive value of  $\mu_k$  is calculated quantum mechanically [13]. Pedri and co-workers [14] have calculated the local chemical potential to be

$$\mu_{k=0} = \left( \frac{\pi^2 (s_x s_y s_z)^{1/3}}{4} \right)^{1/10} \mu_0 \quad (10)$$

where  $\mu_0$  is the chemical potential in the absence of the optical potential.

### 3. Heat capacity

In DOS approach, the heat capacity is calculated by differentiating the internal energy,  $U = k_B T^2 \left( \frac{\partial q}{\partial T} \right)_z$ , with respect to the temperature, i.e.

$$C_V(T) = \left( \frac{\partial U}{\partial T} \right)_{N,V}. \quad (11)$$

However, one has to take into account two different regimes. For  $T < T_0$  the chemical potential  $\mu_{k=0}$  is fixed and the number of atoms in the ground state  $N_0$  depends on the temperature. From equations(11), one has

$$\frac{C(T < T_0)}{Nk_B} = \frac{1}{\gamma^3} \left\{ 12 \left( \frac{T}{T_0} \right)^3 \frac{\zeta(4)}{\zeta(3)} + 6 R \left( \frac{T}{T_0} \right)^2 \right\}, \quad (12)$$

where  $T_0 = \frac{\hbar\Omega}{K_B} \left( \frac{N}{\zeta(3)} \right)^{1/3}$  is the BEC transition temperature for the ideal Bose gas trapped in the harmonic potential. Parameter  $R$  is given by

$$R = \frac{3\bar{\omega}}{2\Omega} \left( \frac{\zeta(3)}{N} \right)^{1/3} + \frac{2}{3} \eta \gamma \frac{\Omega}{\bar{\omega}} \left( \frac{\pi^2 (s_x s_y s_z)^{1/3}}{4} \right)^{1/10}, \quad (13)$$

where  $\eta = \frac{\mu_0}{K_B T_0}$  is a scaling parameter for interaction effect, first introduced by Dalfovo et al. in [15] and calculated in [9]. It is easy to see that parameter  $R$  simultaneously considers the main effects which can alter the ideal Bose gas trapped in the combined potential. The first term gives the finite size effect while the second term accounts for the interatomic interaction and the deepness of the lattice.

For  $T > T_0$ , on the other hand,  $N_0$  vanishes and  $\mu_0$  depends on temperature. Thus the heat capacity for  $T > T_0$  still depends on  $T$  and  $\mu_0$ . The slightly more difficult point here is that  $N$  has to be considered as a fixed and so  $\mu_0$  has to be considered as a function of  $N$  and  $T$ . However the quantity  $\frac{\partial}{\partial \beta}(\beta\mu)$  will be needed in calculating  $C(T > T_0)/Nk_B$ . This quantity can be found from equation (9) given that  $N$  is fixed. Following Grossmann and Holthaus [5], one has

$$\begin{aligned} \frac{C_V(T > T_0)}{Nk_B} &= \frac{1}{\gamma^3} \left\{ \left[ 12 \frac{g_4(z)}{\zeta(3)} \left( \frac{T}{T_0} \right)^3 + 6 \frac{g_3(z)}{\zeta(3)} R \left( \frac{T}{T_0} \right)^2 \right] - \left[ \frac{3g_3(z)}{\zeta(3)} \left( \frac{T}{T_0} \right)^3 \right. \right. \\ &\quad \left. \left. + 2 \frac{g_2(z)}{\zeta(3)} R \left( \frac{T}{T_0} \right)^2 \right] \frac{3g_3(z) + 2R(T_0/T)g_2(z)}{g_2(z) + R(T_0/T)g_1(z)} \right\}. \end{aligned} \quad (14)$$

In absence of the optical potential, i.e.  $\gamma \rightarrow$  unity, the results previously obtained by Crossmann and Holthaus [5] can be obtained by setting  $\eta = 0$  in equation (13). In the thermodynamic limit,  $R = 0$ , and equations (12) and (14) are considerably simplified to

$$\frac{C(T < T_0)}{Nk_B} = \frac{12}{\gamma^3} \frac{\zeta(4)}{\zeta(3)} \left( \frac{T}{T_0} \right)^3 \quad (15)$$

$$\frac{C(T \geq T_0)}{Nk_B} = \frac{3}{\gamma^3} \left[ 4 \frac{g_4(z)}{g_3(z)} - 3 \frac{g_3(z)}{g_2(z)} \right]. \quad (16)$$

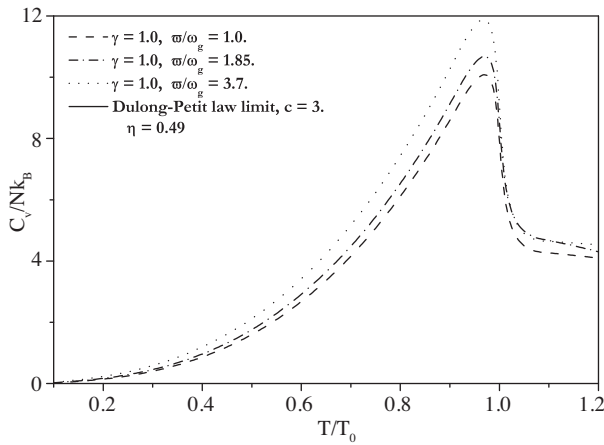
Thus the heat capacity is discontinuous at  $T = T_0$ .

According to the Ehrenfest definition, this discontinuity characterizes the phase transition to be of second order. Furthermore, one observes that the heat capacity, equation (15), obeys the third law of thermodynamics, which demands a vanishing heat capacity at zero temperature, and reproduces the Dulong-Petit law type in the very high temperature limit,  $(C(T \geq T_0)/Nk_B)_{T \rightarrow \infty} = 3\gamma^{-3}$ .

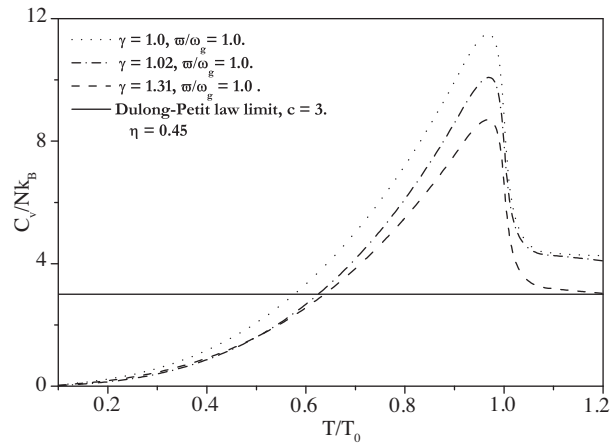
In Figure 1 the results calculated from equations (12) and (14) are plotted for  $\gamma = 1$ . This figure shows that the BEC is accompanied by a peak in the specific heat capacity at temperature equal to the condensation temperature,  $T/T_0 = 1$ , for the isotropic harmonic trap. For anisotropic harmonic trap  $\frac{\bar{\omega}}{\omega_g} = 3.0$ , the peak is shifted to the high temperature range, but less than the transition range  $T_0$ . These results are in agreement with the results obtained by Van Druten and Ketterle [16].

Figure 2 shows that the BEC, in a combined isotropic harmonic potential with anisotropic hopping lattice potential,  $\gamma > 1$ , is accompanied by a peak in the heat capacity. Peaks for the combined isotropic harmonic-lattice potential are at higher temperature than that observed for the anisotropic harmonic potential case. However, this result does not agree with the results of Ramakumar and Das [17] for isotropic harmonic potential. Their numerical calculations showed that when bosons are in an isotropic harmonic with highly anisotropic hopping in the optical lattice, the peak is not shifted.

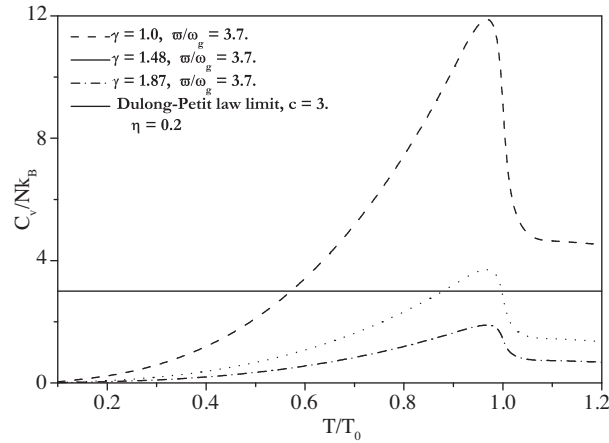
Figure 3 shows that the BEC in a combined anisotropic harmonic potential with anisotropic hopping lattice potential,  $\gamma > 1$ , is also accompanied by a peak in the heat capacity. In the high temperature limit, the heat capacity still reproduces the Dulong-Petit law type.



**Figure 1.** Variation of the specific heat capacity  $C_V/Nk_B$  is plotted against reduced temperature  $T/T_0$ , for harmonically confined bosons in isotropic and anisotropic harmonic traps. The horizontal solid line corresponds to the Dulong-Petit law.



**Figure 2.** Variation of the heat capacity  $C_V/Nk_B$  is plotted against reduced temperature  $T/T_0$ , in a combined isotropic harmonic potential with anisotropic hopping lattice potential. The horizontal solid line corresponds to the Dulong-Petit law.



**Figure 3.** Variation of the heat capacity  $C/Nk_B$  is plotted against reduced temperature  $T/T_0$ , in a combined anisotropic harmonic potential with anisotropic hopping lattice potential. The horizontal solid line corresponds to the Dulong-Petit law.

## 4. Discussion and conclusion

The heat capacity for interacting bosons trapped in a combined harmonic lattice potential has been investigated in this work. Among other results, the heat capacity has a significant dependence on the temperature and the lattice depth. Moreover, it shows a  $\lambda$  anomaly at  $T_0$ , and is accompanied by a peak at the transition temperature. The heat capacity peak's for high lattice depth occurs at lower temperature than that of low lattice depth. This behavior is due to the fact that the transition temperature decreases with the increased lattice depth. There is a discontinuity in the heat capacity, and this discontinuity remains finite for the combined potential. In the thermodynamic limit,  $N \rightarrow \infty$ , the discontinuity becomes smaller by a factor of  $\gamma^{-3}$ . It is interesting to notice that the interaction effect is still visible, even in the presence of the optical potential, but it is strongly quenched. In contrast to previous work, the DOS approach involves only analytical calculations without technical complication.

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