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Two-step condensation of lattice bosons

R. Ramakumar [a,*], A.N. Das [b]

[a] Department of Physics and Astrophysics, University of Delhi, Delhi-110007, India
[b] Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata-700064, India

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ABSTRACT

We present a theoretical study of Bose–Einstein condensation in highly anisotropic harmonic traps. The bosons are considered to be moving in an optical lattice in an overall anisotropic harmonic confining potential. We find that two-step condensation occurs for lattice bosons at much reduced harmonic potential anisotropy when compared to the case of an ideal Bose gas in an anisotropic harmonic confinement. We also show that when the bosons are in an isotropic harmonic confinement but with highly anisotropic hopping in the optical lattice, two-step condensation does not occur. We interpret some of our results using single boson density of energy states corresponding to the potentials faced by the bosons.

1. Introduction

The experimental observation [1–3] of Bose–Einstein (BE) condensation in confined Bose atom clouds have launched extensive experimental and theoretical studies of this phenomenon and the various properties of the condensates of free bosons [4] and lattice bosons [5–10]. In three dimensional non-interacting free [7] or lattice Bose systems [11] in isotropic harmonic traps, the BE condensation is accompanied by a peak in the specific heat at the condensation temperature. However, not long after the initial discovery of Bose condensation in harmonic traps, Druten and Ketterle (DK) [12] found that bosons in highly anisotropic three dimensional (3D) harmonic traps show a qualitatively different behavior of the specific heat. Their theoretical calculations showed that the peak in the specific heat of this system is not at the Bose condensation temperature, but in a higher temperature range in which the bosons, as the temperature decreases, are progressively transferred from the tightly confined dimensions to a loosely confined dimension. Thus, in this system, the Bose condensation occurs in two steps: first the aforementioned transfer and second the condensation of all bosons in to the overall ground state. The calculations of DK are for free bosons in anisotropic 3D harmonic traps. The earlier [13] and the later works [14] are also for free bosons with anisotropic box and anisotropic 3D harmonic confinements, respectively.

The two-step condensation is a phenomenon special in at least two aspects. The first aspect is that the condensation of the bosons into the overall ground state occurs without any signature in a thermodynamic property (the specific heat). The second aspect is that it involves a dimensionality cross-over in a higher temperature range. Both of these aspects are of fundamental importance, and hence an investigation of this phenomenon for *lattice bosons* should be of significant interest. Now, when an additional optical lattice potential is applied to bosons in a harmonic trap, it is known that significant changes occur in the single boson energy density of states (DOS) [11,15,16]. How these changes alter the two-step condensation phenomenon is an issue of fundamental importance and contemporary relevance. Further, considering that there is a dimensionality cross-over involved, it should of interest to know under what conditions a *lattice bosons* system in an anisotropic harmonic trap is truly one-dimensional as far as thermodynamic properties are concerned. Motivated by these considerations, in this paper we present a theoretical study of the condensation of lattice bosons in anisotropic harmonic

* Corresponding author.
E-mail address: rkumar@physics.du.ac.in (R. Ramakumar).

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traps. Among other results, we show that a two-step condensation occurs for lattice bosons at anisotropies much smaller than that required for free bosons. This finding may lead to an experimental study of this phenomenon in optical lattices. Further, since it is by now relatively easy to experimentally change the boson hopping in different spatial directions in an optical lattice, we also study a case of lattice bosons with anisotropic hopping in an isotropic harmonic confining potential. One may argue that this is equivalent to bosons with isotropic hopping in an anisotropic trap and hence two-step condensation would occur in this case as well. Our calculations show that two-step condensation does not occur in this case. Our focus in this paper is the effects of the optical lattice potential on the two-step condensation. We will not consider the effect of boson–boson interactions here for simplicity. Furthermore we will make a tight binding approximation to the optical potential and consider the ground state band. The applicability of the tight binding approximation, the corrections due to excited bands and interactions for a combined harmonic trap and optical potential in various properties of bosons have been discussed by Blakie and Wang [17], Baillie and Blakie [18,19] and others [20,21]. The strength of the boson hopping and interactions, and the band gap between the ground and the excited bands are controllable in optical lattices [9,22] by adjusting the depth of the potential. Experimentally a situation may be reached where the effects of the corrections due to the excited band as well as due to interactions are negligible. In Section 2.2 we would discuss about the possible parameter space where our results are applicable.

This paper is organized as follows. In the next section, we revisit the system of free bosons in an anisotropic harmonic trap. We complement the analysis of DK by new features we find in the single boson density of energy states (DOS). In Section 2, we analyze two-step condensation of lattice bosons in anisotropic harmonic traps. In Section 3, we study the Bose condensation of lattice bosons with anisotropic hopping in an isotropic harmonic trap. The conclusions are given in Section 4.

2. Two-step condensation of free and lattice bosons

2.1. Free bosons in an anisotropic harmonic potential

In this section we consider boson atoms in an anisotropic harmonic confining potential ($K_x x^2 + K_y y^2 + K_z z^2$). The single boson energy levels are $E(n_x, n_y, n_z) = (n_x + 1/2)\hbar\omega_x + (n_y + 1/2)\hbar\omega_y + (n_z + 1/2)\hbar\omega_z$, where $n_x, n_y, n_z = 0, 1, 2, \ldots, \infty$, $2\pi\hbar$ is the Plank's constant, and $\omega_{x,y,z} = \sqrt{2K_{x,y,z}/m}$ in which m is the atomic mass. We use $K_x \ll K_y = K_z$ so that the potentials, from the center of the trap, along the y and z directions are much steeper compared to that along the x direction. In order to exhibit the two-step condensation in this system, we calculate the ground state occupancy (N_0), the occupancy in the loosely confined direction (N_{1D}), and the specific heat by determining first the chemical potential (μ) from the bosons number equation $N = \sum_{n_x=0}^{\infty}\sum_{n_y=0}^{\infty}\sum_{n_z=0}^{\infty} N(E(n_x, n_y, n_z))$, where $N(E) = 1/(\exp[\beta(E-\mu)] - 1)$, $\beta = 1/k_B T$, T the temperature, and then calculating $N_0 = N(E(0,0,0))$ and $N_{1D} = \sum_{n_x=0}^{\infty} N(E(n_x, 0, 0))$. The specific heat is obtained from the temperature derivative [11] of the total energy ($E_{\text{tot}} = \sum_{n_y=0}^{\infty}\sum_{n_z=0}^{\infty}\sum_{n_x=0}^{\infty} N(E(n_x, n_y, n_z))E(n_x, n_y, n_z)$). We evaluated N_0, N_{1D}, and C_v numerically to obtain exact results. The results of our calculations for 10 000 bosons in harmonic traps of varying anisotropies are shown in Fig. 1. The condensation temperature [11,23] (T_0), mentioned in this and other figures, is obtained by setting $N_0 = 0$ and $\mu = E(0,0,0)$ in the bosons number equation. For low anisotropy, the peak in C_v is clearly associated with the growth of the Bose condensate fraction (N_0/N). With increasing anisotropy, the peak in C_v becomes associated with the dimensionality cross-over in which bosons are transferred from the tightly confined directions (y and z) into the loosely confined direction (x). To complement the analysis of DK, we calculated the single boson energy DOS for these systems. First we recall that the analytical approximation to the DOS of a boson in a D-dimensional anisotropic harmonic trap [7] is

$$D(E) = \frac{E^{D-1}}{(D-1)!\prod_{i=1}^{D}(\hbar\omega_i)}. \tag{1}$$

From exact numerical calculations, we find that the DOS for highly anisotropic traps, shown in Fig. 2(a), show features qualitatively different from the analytical approximation. The DOS is found to have a one dimensional (1D) character (flat regions). In the very low temperature range, only the lowest flat region is occupied by bosons so that the C_v shows 1D character as shown in the inset of Fig. 1. This is consistent with the higher temperature cross-over in which the bosons are transferred from the tightly confined directions to the loosely confined direction. We also note that 1D features are absent in the DOS when the anisotropy is comparatively smaller as shown in Fig. 2(b). In the next section, we consider two-step condensation of lattice bosons.

2.2. Lattice bosons in an anisotropic harmonic potential

In this section we consider boson atoms in a three dimensional simple cubic (sc) lattice in an overall anisotropic harmonic confining potential. The system Hamiltonian is

$$H = -t\sum_{\langle ij\rangle}\left(c_i^{\dagger}c_j + c_j^{\dagger}c_i\right) + \sum_i V(i)n_i - \mu\sum_i n_i, \tag{2}$$