Two-step condensation of lattice bosons

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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.

I. INTRODUCTION

The experimental observation\textsuperscript{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\textsuperscript{4} and lattice bosons\textsuperscript{5–10}. In three dimensional non-interacting free\textsuperscript{7} or lattice Bose systems\textsuperscript{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)\textsuperscript{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 boson 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 loosely confined dimension. Thus, in this system, the boson condensation occurs in two steps: first the aforementioned transfer and second the condensation of all bosons into the overall ground state. The calculations of DK are for free bosons in anisotropic 3D harmonic traps. The earlier\textsuperscript{13} and the later works\textsuperscript{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\textsuperscript{11,15,16} (DOS). 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 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, not the effect of boson-boson interactions. The strength of boson interactions is controllable in optical lattices\textsuperscript{9,17}, and hence one can experimentally reach the ideal gas limit to which 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 Sec. II, we analyze two-step condensation of lattice bosons in anisotropic harmonic traps. In Sec.
III, we study the Bose condensation of lattice bosons with anisotropic hopping in an isotropic harmonic trap. The conclusions are given in Sec. IV.

II. TWO-STEP CONDENSATION OF FREE AND LATTICE BOSONS

A. 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 \(n_x, n_y, n_z = 0, 1, 2, \ldots \infty\) 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 \(\mu\) 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 \(N(E) = \frac{1}{\exp[\beta(E - \mu)] - 1}\), \(\beta = 1/k_BT\), \(T\) the temperature, and then calculating \(N_0 = N(E(0,0,0))\) and \(N_{1D} = \sum_{n_z=0}^{\infty} N(E(n_x, n_y, n_z))\). The specific heat is obtained from the temperature derivative\(^{11}\) of the total energy \(E_{tot} = \sum_{n_x=0}^{\infty} \sum_{n_y=0}^{\infty} \sum_{n_z=0}^{\infty} N(E(n_x, n_y, n_z))E(n_x, n_y, n_z))\). We evaluated \(N_0\), \(N_{1D}\), and \(C_v\) numerically to obtain exact results. The results of our calculations for 10000 bosons in harmonic traps of varying anisotropies are shown in Fig. 1. The condensation temperature\(^{11,18}\) \(T_c\), 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 is

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

From exact numerical calculations, we find that the DOS for highly anisotropic traps, shown in Fig. 2a, show features qualitatively different from the analytical approximation. The DOS is found to have 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. 2b. In the next section, we consider consider two-step condensation of lattice bosons.

B. 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

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

where \(t\) is the kinetic energy gain when a boson hop from site \(i\) to its nearest neighbor site \(j\) in the optical lattice, \(c_i^\dagger\) is a boson creation operator, \(V(i) = (K_x x_i^2 + K_y y_i^2 + K_z z_i^2)\) is the potential at site \(i\), \(n_i = c_i^\dagger c_i\) the boson number operator, and \(\mu\) the chemical potential. We numerically diagonalize this hamiltonian to obtain the energy levels \((E_i)\) of a lattice boson for different values of the anisotropy of the harmonic trap with \(k_x \ll k_y = k_z\), where \(k_\alpha = K_\alpha a^2\), \(\alpha = x, y, z\) and \(a\) is the lattice constant of the sc optical lattice. The chemical potential and the boson populations in different energy levels are calculated at a temperature \(T\), using the boson number equation: \(N = \sum_{E_0}^{E_m} N(E_i))\), where \(E_0\) and \(E_m\) are the lowest and the highest single boson energy levels and \(N(E_i) = \frac{1}{\exp[(E_i - \mu)/k_BT] - 1}\). The specific heat is calculated from the temperature derivative of total energy \(E_{tot} = \sum_{i=0}^{E_m} N(E_i)E_i\). The lattice size, we use, is large enough that the results are free of finite size effects. The results for the temperature dependence of the Bose condensate fraction \(N_0/N\), fractional boson population in the \(x\)-direction \((N_{1D}/N)\), and the specific heat
for lattice bosons in harmonic traps with different anisotropies are shown in Fig. 3. The two-step condensation is clearly seen in highly anisotropic traps (dash-dot and dotted lines), while it is absent for small anisotropies. Further, on comparing Figs. 1 and 3, we can immediately infer that the two-step condensation of lattice bosons is possible for much smaller anisotropies compared to the free bosons in anisotropic harmonic traps. We also find that most of the lattice bosons are confined in the \(x\)-direction at much higher temperatures compared to the case of free bosons even though the anisotropy is much smaller for the former compared to the latter. This is clear if we compare \(N_{1D}/N\) in both cases, as shown in Figs. 1 and 3, for \(T > 2.5T_0\). In order to get some insight into the two-step condensation occurring for smaller anisotropies for lattice bosons, we calculated the single boson energy DOS for these systems. The results of our calculations are shown in Fig. 4. With increasing anisotropy there is a dramatic change in the single particle DOS (Fig. 4). Except for very low energies, the DOS for low anisotropy is very similar to that for the isotropic case. With increasing anisotropy, the DOS develops features similar to that expected in 1D. It has peaks separated by broad regions of comparatively very small values of DOS. Since the DOS shows strong 1D features for small anisotropies compared to the free boson case (without the lattice potential), the 1D behavior in \(N_{1D}/N\) sets in for comparatively smaller anisotropies of the harmonic traps.

C. Dimensionality cross-overs of lattice bosons

In this section, we investigate the dimensionality cross-over in some more detail. The specific heat, being a very sensitive function of dimensionality changes, is an useful property to study for this purpose. As mentioned earlier, for bosons in a highly anisotropic harmonic trap, the peak in the specific heat occurs in a temperature range in which the bosons are transferred from the tightly confined directions to the loosely confined direction (here \(x\)-direction passing through the center of the trap). With lowering of temperature, when the transfer to the single 1D chain along the \(x\)-direction is complete, the system would show 1D behavior. To visualize this cross-over, we have plotted the specific heats of lattice bosons in 3D anisotropic traps and in a 1D trap in Fig. 5. It is seen that at low temperatures the specific heats of the anisotropic systems completely coincide with that of the 1D chain showing that the anisotropic 3D systems have become purely 1D. The departure from the 1D behavior starts at a temperature which is higher for larger anisotropy (Fig. 5). However, this temperature is much lower than the temperature where the specific heat shows the peak and is also lower than the condensation temperature \((T_0)\) for anisotropic as high as \(k_y/k_z = 2 \times 10^5\) for lattice bosons (see Fig. 5). It is also found that above this temperature (i.e., where the departure from the 1D behavior starts in \(C_v\)), a very small change in \(N_{1D}\) produces a very large change in \(C_v\). This is also clear from Fig. 1 (for free bosons) and from Figs. 3 and 5 (for lattice bosons) on comparing the temperature dependences of \(C_v\) and \(N_{1D}\) in the above mentioned region.

III. LATTICE BOSONS WITH ANISOTROPIC HOPPING IN AN ISOTROPIC HARMONIC POTENTIAL

In this section, we investigate if the properties of lattice bosons with anisotropic hopping in an isotropic harmonic trap is similar to those with isotropic hopping in an anisotropic harmonic trap. We have studied the effects of anisotropic hopping on \(C_v\) and condensate fraction in isotropic harmonic traps. The spatial direction dependent hopping we use are such that \(t_x \gg t_y = t_z\). The results of our calculations for various anisotropy ratios are shown in Fig. 6. We do not find a two-step behavior in this system. The specific heat is suppressed with increasing hopping anisotropy. The system shows anisotropic 3D behavior in all the properties studied even for large hopping anisotropies.

The reason is that even though the hopping is anisotropic, since the trap is isotropic, one will have a large collection of 1D chains, symmetric about the central one, coupled by the small inter-chain hopping. At the boson condensation temperature, the bosons condense in to the central region of the trap. There is no higher temperature cross-over region as in the case of lattice bosons with isotropic hopping in a highly anisotropic harmonic trap.

IV. CONCLUSIONS

In this paper we presented a theoretical study of two-step condensation of lattice bosons in anisotropic harmonic confining potentials. We find that, even though significant changes occur in the single bosons DOS, two-step condensation occurs for lattice bosons and it occurs for much smaller anisotropies of the harmonic potential compared to that for free bosons. This may lead to experimental observation of these type of condensations. We find unusual 1D features in the one boson DOS both for free and lattice bosons in highly anisotropic harmonic traps. These DOS's
are equally well applicable to fermions. Using $C_v$ as the indicator, we also investigated the dimensionality cross-overs in the system. We find that the system shows purely 1D behavior in a much lower temperature range compared to the temperature range in which the peak in $C_v$ occurs. Further, we investigated if two-step condensation occurs for lattice bosons with anisotropic hopping in an isotropic harmonic trap. We find that a two-step condensation does not occur in this system.

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FIG. 1. The variation of the specific heat ($C_v$), bose condensate fraction ($N_0/N$), and the fractional population in the $x$-direction ($N_{1D}/N$) with temperature for free bosons in anisotropic harmonic traps. $T_0$ is the condensation temperature as defined in the text. Solid line: $K_x = 0.01$, $K_y = K_z = 10$, dotted line: $K_x = 0.01$, $K_y = K_z = 1000$, and dash-dot line: $K_x = 0.01$, $K_y = K_z = 50000$. In our energy units $\hbar\omega_x = 0.1414$, whereas $\hbar\omega_y (= \hbar\omega_z) = 4.47, 44.72,$ and 316.2 for $K_y = 10, 1000,$ and 50000, respectively. The number of bosons ($N$) used is 10000. The inset shows a comparison between $C_v$'s of an anisotropic case (dotted lines for $K_x = 0.01$, $K_y = K_z = 50000$) and a pure 1D case (solid line) with $K_x = 0.01$. 
FIG. 2. The single particle DOS for free bosons in an anisotropic harmonic trap vs energy E. Top panel (a): $K_x = 0.01$ and $K_y = K_z = 50000$; triangles give the numerically calculated exact DOS, dashed line is the DOS obtained from the analytical expression in Eq. 1. Bottom panel (b): $K_x = 0.01$ and $K_y = K_z = 10$; thin solid line represents numerically calculated exact DOS, dashed line is the DOS obtained from Eq. 1. In our energy unit $\hbar \omega_x = 0.1414$. 
FIG. 3. The variation of the specific heat ($C_v$), bose condensate fraction ($N_0/N$), and the fractional population in the $x$-direction ($N_{1D}/N$) with temperature for bosons in combined optical lattice and anisotropic harmonic potentials. Solid line: $k_x = 0.01$, $k_y = k_z = 10$, dotted line: $k_x = 0.01$, $k_y = k_z = 100$, and dash-dot line: $k_x = 0.01$, $k_y = k_z = 1000$ (in units of $t = 1$). The number of bosons ($N$) used is 10000.
FIG. 4. The single particle DOS for bosons in combined optical lattice \((t = 1)\) and different anisotropic harmonic potentials. Circles: \(k_x = 0.01, k_y = k_z = 10\) and solid line: \(k_x = 0.01, k_y = k_z = 1000\).
FIG. 5. Comparison of the specific heat ($C_v$) of 10000 bosons in the 3D anisotropic harmonic and optical lattice potentials with that of bosons in a 1D combined harmonic and optical lattice. Dotted line: $k_x = 0.01, k_y = k_z = 1000$, dash line: $k_x = 0.01, k_y = k_z = 2000$, and dash-dot line: $k_x = 0.01, k_y = k_z = 4000$ (in units of $t = 1$). The solid line is for a 1D lattice with $k_x = 0.01$. 
FIG. 6. The variation of the specific heat ($C_v$), bose condensate fraction ($N_0/N$), and the fractional population in the $x$-direction ($N_{1D}/N$) with temperature for bosons in combined isotropic harmonic ($k_x = k_y = k_z = 0.01$) and anisotropic optical lattice potentials. Solid line: $t_y = t_z = 1.0$, dotted line: $t_y = t_z = 0.01$, and dash-dot line: $t_y = t_z = 0.001$ (all energy parameters are in units of $t_x = 1.0$). The number of bosons ($N$) used is 10000.