

Bose-Einstein condensation in tight-binding bands

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(Received 22 October 2004; revised manuscript received 11 July 2005; published 2 September 2005)

We present a theoretical study of the condensation of bosons in tight-binding bands corresponding to simple cubic, body-centered cubic, and face-centered cubic lattices. We have analyzed noninteracting bosons, weakly interacting bosons using the Bogoliubov method, and strongly interacting bosons through a renormalized Hamiltonian approach valid for the number of bosons per site less than or equal to unity. In all the cases studied, we find that bosons in a body-centered cubic lattice have the highest Bose condensation temperature. The growth of the condensate fraction of noninteracting bosons is found to be very close to that of free bosons. The interaction partially depletes the condensate at zero temperature and close to it, while enhancing it beyond this range below the Bose-Einstein condensation temperature. Strong interaction enhances the boson effective mass as the band-filling is increased and eventually localizes the bosons to form a Bose-Mott-Hubbard insulator for integer filling.

DOI: [10.1103/PhysRevB.72.094301](https://doi.org/10.1103/PhysRevB.72.094301)

PACS number(s): 03.75.Lm, 03.75.Nt, 03.75.Hh, 67.40.-w

I. INTRODUCTION

In a many-boson system, when the thermal de Broglie wavelength of a particle becomes comparable to the interparticle separation, a condensation in momentum space occurs at a finite temperature and a macroscopic number of particles occupy the lowest single-particle energy level and enter into a phase-locked state. This phenomenon predicted by Einstein¹ by applying Bose statistics² to a three-dimensional homogeneous system of noninteracting atoms in the thermodynamic limit is well known as the Bose-Einstein condensation. Although it took 70 years to eventually observe Bose-Einstein condensation³⁻⁶ in metastable, inhomogeneous, finite, and three-dimensional Bose atom vapors, progress ever since has been tremendous. Extensive investigations of various aspects of the condensate, a macroscopic quantum coherent state of atoms, is now a rapidly expanding field of research.⁷⁻¹¹

One of the interesting recent developments in this field is the observation,¹² by Greiner and collaborators, of a transition between superfluid and Mott insulating phases of bosons in an optical lattice. Researchers have explored this superfluid-Mott transition and the excitation spectra in the superfluid^{12,13} and Mott insulating phases.¹² In these experiments, the condensate is adiabatically transferred to a simple-cubic optical lattice produced by counterpropagating laser beams. By changing the characteristics of the laser beams, it has been possible to achieve great control over t/U , where t is the intersite hopping energy and U the on-site boson-boson interaction energy. It has been shown that bosons in optical lattices can be adequately modeled by employing a clean Bose-Hubbard model.¹⁴ That a bandwidth-controlled transition from a superfluid state to a Bose-Mott-Hubbard (BMH) insulating state is possible at a critical value of t/U for integer number of bosons per site was predicted in theoretical studies¹⁴⁻¹⁹ on the Bose-Hubbard model. In the BMH insulator, the bosons are site localized and the single-particle excitation spectrum acquires a gap. Recently, superfluid to Mott insulator transition was observed²⁰ in finite one-dimensional optical lattices as well.

The experimental realization of bosons in optical lattices provides a microscopic laboratory for the exploration of the collective behavior of quantum many-particle systems in narrow energy bands with great control on t , U , and the number of boson per site (n). There are already theoretical studies^{21,22} on the possibility of creating different types of two-dimensional lattices (triangular, square, and hexagonal, for example). It has been proposed²³ recently that a trimerized optical Kagome lattice can be achieved experimentally and that a superfluid-Mott transition at fractional filling is possible for bosons in this lattice. It is reasonable to expect that three- and two-dimensional optical lattices of different symmetries will be created in the near future. Many experimental groups have produced three-dimensional optical lattices, and experimental studies of Bose condensates in these lattices will surely receive increasing attention. Motivated by such possibilities, we present a theoretical study of Bose-Einstein condensation in tight-binding bands corresponding to simple cubic (sc), body-centered cubic (bcc), and face-centered cubic (fcc) lattices. We have analyzed noninteracting, weakly interacting, and strongly interacting bosons. The weakly interacting bosons were analyzed using a Bogoliubov type theory.²⁴ For the strongly interacting bosons, we use a renormalized Hamiltonian valid for $n \leq 1$ obtained by projecting out on-site multiple occupancies. This analysis is presented in the next section, and the conclusions are given in Sec. III.

II. BOSE CONDENSATION IN TIGHT-BINDING BANDS

A. Noninteracting bosons

In this section, we discuss the simplest of the three cases studied. The Hamiltonian of the noninteracting bosons in a tight-binding energy band is

$$H = \sum_{\mathbf{k}} [\epsilon(\mathbf{k}) - \mu] c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}, \quad (1)$$

where $\epsilon(\mathbf{k})$ is the band structure corresponding to sc, bcc, and fcc lattices, μ the chemical potential, and $c_{\mathbf{k}}^{\dagger}$ is the boson

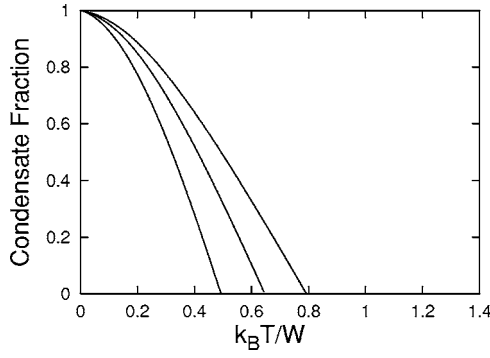


FIG. 1. The variation of the condensate fraction with temperature for bosons in a sc lattice for $n=0.8$ (top), $n=0.6$ (middle), and $n=0.4$ (bottom). In this and later figures, W is the half-bandwidth.

creation operator. Confining to nearest-neighbor Wannier function overlaps, these band structures when lattice constant is set to unity are

$$\begin{aligned} \epsilon_{sc}(k_x, k_y, k_z) &= -2t \sum_{\mu=x}^z \cos(k_\mu), \\ \epsilon_{bcc}(k_x, k_y, k_z) &= -8t \prod_{\mu=x}^z \cos\left(\frac{k_\mu}{2}\right), \end{aligned} \quad (2)$$

and

$$\epsilon_{fcc}(k_x, k_y, k_z) = -2t \sum_{\mu=x; \mu \neq \nu}^z \sum_{\nu=x}^z \cos\left(\frac{k_\mu}{2}\right) \cos\left(\frac{k_\nu}{2}\right), \quad (3)$$

where t is the nearest-neighbor boson-hopping energy. The condensation temperature (T_B) for bosons in these bands can be calculated from the boson number equation

$$n = \frac{1}{N_x N_y N_z} \sum_{k_x} \sum_{k_y} \sum_{k_z} \frac{1}{e^{[\epsilon(k_x, k_y, k_z) - \mu]/k_B T} - 1}, \quad (4)$$

where $N_s = N_x N_y N_z$ is the total number of lattice sites, k_B the Boltzmann constant, and T the temperature. At high temperature, the chemical potential is large and negative. As the temperature comes down, the chemical potential raises gradually to eventually hit the bottom of the band. Below

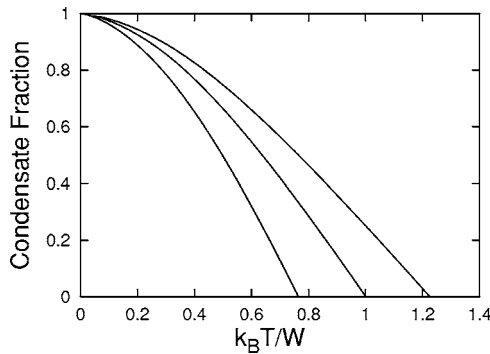


FIG. 2. The same as in Fig. 1 for bosons in a bcc lattice for $n=0.8$ (top), $n=0.6$ (middle), and $n=0.4$ (bottom).

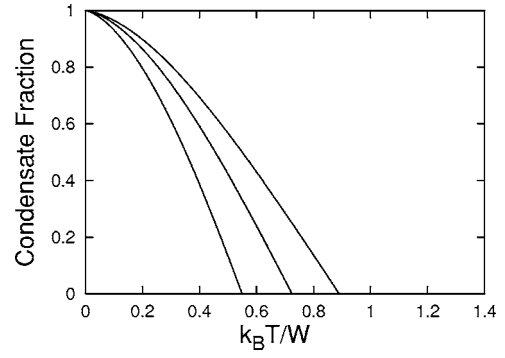


FIG. 3. The same as in Fig. 1 for bosons in a fcc lattice for $n=0.8$ (top), $n=0.6$ (middle), and $n=0.4$ (bottom).

this temperature, there is macroscopic occupation of the band bottom, and we have a Bose condensate. On further reduction of temperature, the chemical potential is pinned to the bottom of the band, and bosons are progressively transferred from excited states into the condensate. All the particles are in the condensate at absolute zero temperature. Fixing the chemical potential at the bottom of the band, the solution of the number equation gives the Bose condensation temperature (T_B). For $T > T_B$, a lower value of μ satisfies the number equation, while for $T < T_B$, the right-hand side of Eq. (4) is less than the number of bosons (n), the difference being the number of condensate particles (n_0). We determined T_B and n_0 for different lattices as a function of filling and temperature. Results of these calculations are shown in Figs. 1–5. We find that bosons in the tight-binding band corresponding to the bcc lattice have the highest Bose condensation temperature. Comparing the single boson density of states (DOS), we find that the band structure with smallest DOS near the bottom of the band has the highest T_B . The physical reason behind it is that, as the temperature is lowered from above the Bose condensation temperature, the bosons are transferred from the high-energy states to the low-energy states following the Bose distribution function. To accommodate these bosons, the chemical potential would touch the bottom of the boson band at a higher temperature for a system with smaller DOS near the bottom of the band compared to a system that has larger DOS there. Consequently, the Bose condensation temperature for the former system would be

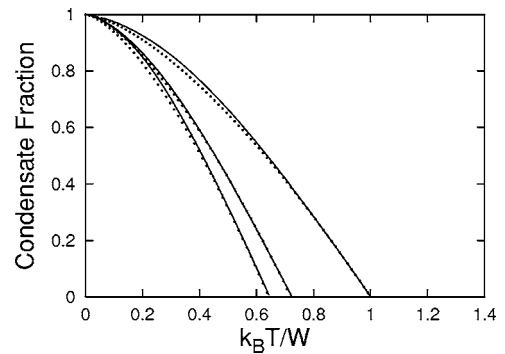


FIG. 4. The variation of the condensate fraction (for $n=0.6$) for bcc (top), fcc (middle), and sc (bottom) lattices. The dots are plots of $1 - (T/T_c)^{3/2}$.

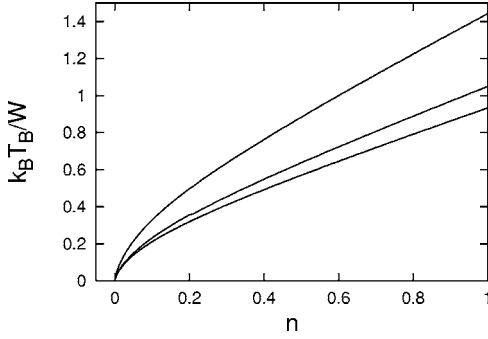


FIG. 5. The variation of the Bose condensation temperature (of noninteracting or weakly interacting bosons) with n for bcc (top), fcc (middle), and sc (bottom) lattices.

higher than that for the latter. The growth of the condensate fraction for different lattices is shown in Figs. 1–3, and in Fig. 4, we have compared condensate fraction growth for different lattices. Also shown by dotted lines is the condensate fraction for free bosons, which are found to be rather close. The variation of T_B with n is shown in Fig. 5, which shows an initial fast growth and a monotonic increase for higher values of n .

B. Weakly interacting bosons

To study Bose condensation of weakly interacting Bosons in tight-binding bands, we employ the following Hamiltonian:

$$H = \sum_{\mathbf{k}} [\epsilon(\mathbf{k}) - \mu] c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \frac{U}{2N_s} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \sum_{\mathbf{q}} c_{\mathbf{k}+\mathbf{q}}^{\dagger} c_{\mathbf{k}'-\mathbf{q}}^{\dagger} c_{\mathbf{k}'} c_{\mathbf{k}}. \quad (5)$$

Here $\epsilon(\mathbf{k})$ is the boson band structure, μ the chemical potential, $c_{\mathbf{k}}^{\dagger}$ the boson creation operator, U the boson-boson repulsive interaction energy (taken to be a constant for simplicity), and N_s the number of lattice sites. In this section, we will deal with a range of U such that $U < 2W$, where W is the half-bandwidth. Our aim is to get a boson number equation in terms of $\epsilon(\mathbf{k})$, U , μ , and temperature. One can then calculate the condensate fraction and the transition temperature. To this end we follow the Bogoliubov theory.²⁴ In this theory, one makes an assumption that the ground state of interacting bosons is a Bose condensate. Since the lowest single-particle state (which is $\mathbf{k}=0$ in our case of simple tight-binding bands) has macroscopic occupation (say, N_0), we have $\langle c_0^{\dagger} c_0 \rangle \approx \langle c_0 c_0^{\dagger} \rangle$. Then, the operators c_0^{\dagger} and c_0 can be treated as complex numbers, and one gets $\langle c_0^{\dagger} \rangle = \langle c_0 \rangle = \sqrt{N_0}$. This complex number substitution has been recently shown²⁵ to be justified. Clearly, we have a two-fluid system consisting of two subsystems of condensed and noncondensed bosons. There are interactions between particles within each subsystem and interactions between particles in the two subsystems. In the Bogoliubov approach, to obtain second-order interaction terms, one makes the substitution: $c_0^{\dagger} \rightarrow \sqrt{N_0} + c_0^{\dagger}$. In the ground state, the linear fluctuation terms must vanish, and this fixes the chemical potential to $\mu = Un_0 + \epsilon_0$, where ϵ_0

is the minimum of the single-particle energy spectrum (which is equal to $-zt$ for a bipartite lattice with coordination number z), and $n_0 = N_0/N_s$. After a mean-field factorization of the interaction term, we obtain for lattices with inversion symmetry the following mean-field Hamiltonian:

$$H_{BMF} = -E_0 + \sum_{\mathbf{k}}' \frac{\xi(\mathbf{k}) + Un_0}{2} (c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + c_{-\mathbf{k}}^{\dagger} c_{-\mathbf{k}}) + \frac{Un_0}{2} \sum_{\mathbf{k}}' (c_{\mathbf{k}}^{\dagger} c_{-\mathbf{k}}^{\dagger} + c_{-\mathbf{k}} c_{\mathbf{k}}), \quad (6)$$

where $E_0 \equiv -Un_0 N_0/2$ and $\xi(\mathbf{k}) \equiv \epsilon(\mathbf{k}) - \epsilon_0$. As mentioned earlier, our aim is to get an equation for the number of particles. This can be obtained from the Green's function²⁶ $G(\mathbf{k}, \omega) \equiv \langle\langle c_{\mathbf{k}}; c_{\mathbf{k}}^{\dagger} \rangle\rangle_{\omega}$ using the relation

$$n_{\mathbf{k}} = \lim_{\eta \rightarrow 0} \int_{-\infty}^{\infty} [G(\mathbf{k}, \omega + i\eta) - G(\mathbf{k}, \omega - i\eta)] f(\omega) d\omega, \quad (7)$$

where $f(\omega) = 1/[\exp(\omega/k_B T) - 1]$. The Heisenberg equation of motion for $G(\mathbf{k}, \omega)$ is

$$\omega G(\mathbf{k}, \omega) = [c_{\mathbf{k}}, c_{\mathbf{k}}^{\dagger}] + \langle\langle [c_{\mathbf{k}}, H]; c_{\mathbf{k}}^{\dagger} \rangle\rangle_{\omega}, \quad (8)$$

where H is the Hamiltonian of the system. Using H_{BMF} , we obtain

$$\omega G(\mathbf{k}, \omega) = 1 + [\xi(\mathbf{k}) + Un_0] G(\mathbf{k}, \omega) + Un_0 F(\mathbf{k}, \omega), \quad (9)$$

and the Green's function to which $G(\mathbf{k}, \omega)$ is coupled, $F(\mathbf{k}, \omega) \equiv \langle\langle c_{-\mathbf{k}}^{\dagger}; c_{\mathbf{k}}^{\dagger} \rangle\rangle_{\omega}$, obeys the equation of motion

$$\omega F(\mathbf{k}, \omega) = -[\xi(\mathbf{k}) + Un_0] F(\mathbf{k}, \omega) - Un_0 G(\mathbf{k}, \omega). \quad (10)$$

Solving the preceding two equations, one obtains

$$G(\mathbf{k}, \omega) = \left(-\frac{\omega + \xi(\mathbf{k}) + Un_0}{2E(\mathbf{k})} \right) \left(\frac{1}{\omega + E(\mathbf{k})} - \frac{1}{\omega - E(\mathbf{k})} \right), \quad (11)$$

where the Bogoliubov quasiparticle energy $E_{\mathbf{k}}$ is

$$E(\mathbf{k}) = \sqrt{\xi^2(\mathbf{k}) + 2Un_0 \xi(\mathbf{k})}. \quad (12)$$

Note that for the tight-binding band dispersions used, $E(\mathbf{k})$ is linear in \mathbf{k} in the long wave-length limit. Now, the number of particles per site (n) is readily obtained using Eqs. (7) and (11) to be

$$n = n_0 + \frac{1}{2N_s} \sum_{\mathbf{k}}' \left[\left(1 + \frac{\xi(\mathbf{k}) + Un_0}{E_{\mathbf{k}}} \right) \frac{1}{e^{\beta E(\mathbf{k})/k_B T} - 1} \right] + \frac{1}{2N_s} \sum_{\mathbf{k}}' \left[\left(1 - \frac{\xi(\mathbf{k}) + Un_0}{E_{\mathbf{k}}} \right) \frac{1}{e^{-\beta E(\mathbf{k})/k_B T} - 1} \right]. \quad (13)$$

It is useful to look at some limits of the preceding equation. When $U=0$ and $T=0$, we have $n_0=n$, which means that all the particles are in the condensate at absolute zero in the noninteracting limit. When $U=0$ and $T \neq 0$, one obtains

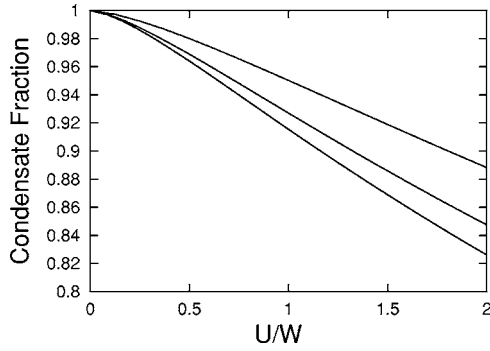


FIG. 6. The variation of the condensate fraction (for $T=0$ and $n=0.4$) with U/W for bcc (top), fcc (middle), and sc (bottom) lattices.

$$n_0 = n - \frac{1}{N_s} \sum_{\mathbf{k}}' \frac{1}{e^{\xi(\mathbf{k})/k_B T} - 1}. \quad (14)$$

The second term on the right-hand side of the preceding equation is the thermal depletion of the condensate. Further, when $U \neq 0$ and $T=0$, we get

$$n_0 = n - \frac{1}{N_s} \sum_{\mathbf{k}}' \left(\frac{\xi(\mathbf{k}) + Un_0 - E(\mathbf{k})}{2E(\mathbf{k})} \right), \quad (15)$$

in which the second term on the right-hand side is the interaction-induced depletion of the condensate. The interaction has twin effects of leading to a modified excitation spectrum and to a partial depletion of the condensate. The gapless and linear long-wavelength excitation spectrum is consistent with experimental measurements¹² on interacting bosons in their Bose-condensed state in optical lattices. In Fig. 6, we have shown the numerical solution of Eq. (13) for bcc, fcc, and sc lattices. The condensate fraction (n_0/n) is seen to be gradually suppressed with increasing U/W . Note also that at $U=0$, all the particles are in the condensate. Finally, we consider the case $U \neq 0$ and $T \neq 0$. In Fig. 7, we have displayed the variation of the condensate fraction as a function of temperature for various values of U/W . The interaction partially depletes the condensate at zero temperature and close to it, while enhancing it beyond this range below the Bose-Einstein condensation temperature. We have not plotted

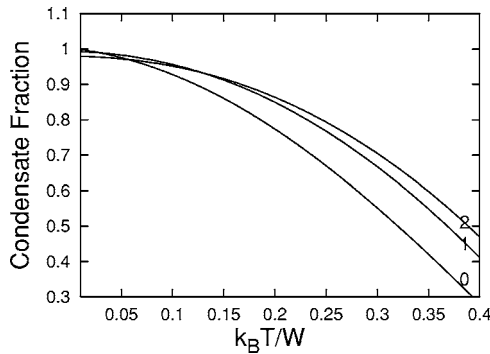


FIG. 7. Condensate fraction (for $n=0.4$) vs temperature for various values of U/W (shown on the curves) and for the sc lattice.

these curves all the way to T_B , since the Bogoliubov approximation breaks down close to T_B . The variation of T_B with n is the same as in the case of noninteracting bosons, as can be seen by setting $n_0=0$ in Eq. (13). At very low temperature, thermal depletion is negligible, and correlation-induced depletion causes a reduction of n_0 with increasing U . At higher temperatures when thermal depletion is important, U plays another role. The energies of the excited states shift to larger values with increasing U ; consequently, the population in the excited states decreases and an enhancement of n_0 occurs with increasing U .

The analysis presented in this section is reasonable provided the effect of interaction is perturbative. When the interaction strength increases, there is a possibility for a correlation-induced localization transition for interacting bosons in a narrow band. In the next section, we analyze this strongly interacting bosons case.

C. Strongly interacting bosons

We first write the Hamiltonian, Eq. (5), in real space. Then we have

$$H = \sum_{ij} (-t - \mu \delta_{ij}) c_i^\dagger c_j + \frac{U}{2} \sum_i n_i(n_i - 1), \quad (16)$$

where $n_i = c_i^\dagger c_i$. For simplicity, let us confine to the case of $n \leq 1$. The effect of increasing interaction (U) is to make the motion of the bosons in the lattice correlated so as to avoid multiple occupancy of the sites. In the dilute limit, the effect of U is not serious since there are enough vacant sites. The effect of U then is prominent when n is close to unity or to an integer value in the general case. In the large U limit, it becomes favorable for the bosons to localize on the sites to avoid the energy penalty of multiple-site occupancy. Qualitatively then, one can see that increasing U increases the effective mass (or decreases the bandwidth) of the bosons and eventually drives them, for integer filling, to a BMH insulator state. For large U , when the double or multiple occupancy is forbidden, one can calculate the bandwidth reduction factor [$\phi_B(n)$] approximately following the spirit of the renormalized Hamiltonian approach (RHA) to the fermion Hubbard model^{27,28} based on the Gutzwiller approximation.^{29,30} Within the RHA, the effect of projecting out double or multiple occupancies on a noninteracting boson wave function is taken into account by a classical renormalization factor that is the ratio of the probabilities of the corresponding physical process in the projected and unprojected spaces. The probability of a hopping process in the projected space is given by $n(1-n)$ for $n \leq 1$. This simply implies that the site from which hopping takes place must be occupied, and the target site must be empty in the projected space. In the unprojected space, the probability of hopping is just equal to the probability of the site from which hopping takes place being occupied. The hopping takes place for noninteracting bosons irrespective of the target site being empty or occupied by any number of bosons. This probability may be found out by calculating the number of ways a given number of noninteracting bosons is distributed in N_s number of lattice sites and (N_s-1) number of lattice sites. The dif-

ference would give the number of configurations where a particular site is occupied. Following this route, the probability that a site is occupied is obtained as:

$$p(N;N_s) = 1 - \frac{(N+N_s-2)!(N_s-1)!}{(N_s-2)!(N+N_s-1)!}, \quad (17)$$

where N and N_s are the total number of bosons and lattice sites, respectively. In the thermodynamic limit

$$p(n) = \frac{n}{1+n}. \quad (18)$$

So, the hopping probability is just $p(n)$. The preceding equation is valid for any n . Now, in the strongly correlated state (large U limit), confining to the case of $n \leq 1$, the hopping probability is $n(1-n)$. Hence, the $\phi_B(n)$ is obtained to be

$$\phi_B(n) = 1 - n^2. \quad (19)$$

The preceding equation is valid only for $n \leq 1$ and in the large U limit. It may be interesting to note that, in the fermion case, $\phi_F(n) = 2(1-n)/(2-n)$, which has been used in the studies³¹ of superconductivity in the strong-coupling fermion Hubbard model of high-temperature superconductors. Since in the large U limit, double or higher site occupancies are forbidden, one can write a renormalized Hamiltonian, valid for $n \leq 1$, for strongly correlated bosons as

$$H_{sc} = \sum_{\mathbf{k}} [\phi_B(n)\epsilon(\mathbf{k}) - \mu]c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}. \quad (20)$$

The preceding H_{sc} is clearly the Hamiltonian of noninteracting bosons in a narrow band that has undergone a strong correlation-induced, filling-dependent band narrowing. One can see that as n increases from 0 to 1, the boson effective mass increases to eventually diverge at $n=1$, and a BMH insulator obtains. We do admit that there are limitations to this renormalized Hamiltonian approach. While it has the advantage that detailed band structure information can be incorporated in the Bose condensation temperature calculation, it has the disadvantage that we have to restrict ourselves to large U and $n \leq 1$. The preceding Hamiltonian is valid for $U/W > (U/W)_c$, where $(U/W)_c$ is the critical value for transition into the Mott insulating phase for $n=1$. Fixing a precise lower limit on (U/W) is not possible in the absence of either exact analytical or numerical solution of the three-dimensional Bose-Hubbard model. It should be mentioned that in this large U limit and for $n \leq 1$, the Bose-Hubbard model is reduced to the lattice Tonks (hard-core boson) gas, which is different from the classical gas of elastic hard spheres investigated by Tonks.³² Our results imply then that the effective mass of bosons in a lattice Tonks gas in a narrow energy band is strongly band-filling dependent. The variation of Bose condensation temperatures with n for bosons with correlation-induced renormalized energy bands corresponding to sc, bcc, and fcc lattices are displayed in Fig. 8. In the region between each curve and the n axis, the bosons are in their Bose-condensed state, and above each curve, they are in their normal state (except at $n=1$ and below $k_B T \approx U$). The variation of T_B is a result of the combined effects of increasing density and increasing effective mass,

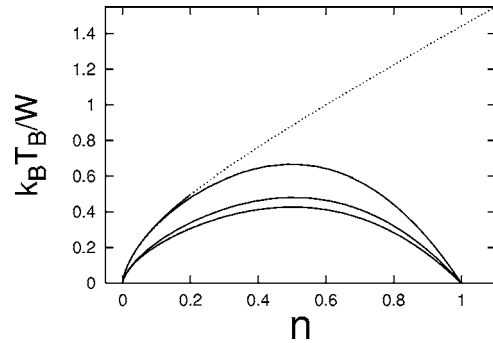


FIG. 8. Bose condensation temperature (of strongly interacting bosons) vs n for bcc (top), fcc (middle), and sc (bottom) lattices. The dots represent noninteracting bosons in a bcc lattice.

since T_B is proportional to n/m^* . Beyond around 20% filling, the increasing effective mass overcompensates the effect of increasing n and pulls down the growth of T_B , eventually driving it to zero at $n=1$, at which density one has a BMH insulator.

It is of some interest to make a comparison between Mott-Hubbard (MH) metal-insulator transitions observed in fermion systems in condensed-matter physics. For a half-filled narrow band of fermions, one way to induce a MH insulator to metal transition is by reducing the ratio of Coulomb repulsion (U) to the bandwidth ($2W$). This was experimentally achieved³³ in V_2O_3 by application of pressure. This then is a bandwidth-controlled MH transition.³⁴ Another way to induce a MH insulator to metal transition is to start with a Mott insulator and reduce the band filling, which would then be a filling-controlled MH transition. This was achieved³⁵ in $La_xSr_{1-x}TiO_3$. For a simple Gutzwiller approximation-based analysis of the properties of this material, see Ref. 36. Now, the Mott transition observed¹² in boson systems in optical lattices is the bandwidth-controlled one. It would be interesting to look for filling-controlled Mott transitions in boson systems in optical lattices that may be possible by starting with the BMH insulator and flipping a few atoms out of the trap.

III. CONCLUSIONS

In this paper, we presented a theoretical study of condensation of bosons in tight-binding bands corresponding to sc, bcc, and fcc lattices. We analyzed condensation temperature and condensate fraction of noninteracting bosons, weakly interacting bosons using the Bogoliubov method, and strongly interacting bosons through a renormalized Hamiltonian approach (limited to $n \leq 1$) capable of incorporating the detailed boson band structures. In all the cases studied, we find that bosons in a tight-binding band corresponding to a bcc lattice have the highest Bose condensation temperature. The growth of the condensate fraction of noninteracting bosons is found to be very close to that of free bosons. In the case of weakly interacting bosons, the interaction partially depletes the condensate at zero temperature and close to it, while enhancing it beyond this range below the Bose-Einstein condensation temperature. Strong interaction enhances the boson effective mass as the band filling is increased and eventually

localizes the bosons to form a Bose-Mott-Hubbard insulator for $n=1$. In the strongly interacting bosons case, we found that all bosons are in the condensate at absolute zero temperature. We also pointed out a possibility of a filling-controlled BMH transition for bosons in optical lattices.

ACKNOWLEDGMENTS

We thank Professor R. K. Moitra for many useful discussions. We also thank Professor Bikas Chakrabarti for a useful discussion.

*On lien from SINP, Kolkata.

- ¹A. Einstein, Sitzungsber. K. Preuss. Akad. Wiss. 261 (1924); 3 (1925).
- ²S. N. Bose, Z. Phys. **26**, 178 (1924).
- ³M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Weiman, and E. A. Cornell, Science **269**, 198 (1995).
- ⁴K. 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).
- ⁵C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet, Phys. Rev. Lett. **75**, 1687 (1995).
- ⁶D. G. Fried, T. C. Killian, L. Willmann, D. Landhuis, S. C. Moss, D. Kleppner, and T. J. Greytak, Phys. Rev. Lett. **81**, 3811 (1998).
- ⁷F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999).
- ⁸A. J. Leggett, Rev. Mod. Phys. **73**, 307 (2001).
- ⁹J. R. Anglin and W. Ketterle, Nature **416**, 211 (2002).
- ¹⁰C. J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge, England, 2002).
- ¹¹D. S. Hall, Am. J. Phys. **71**, 649 (2003).
- ¹²M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature **415**, 39 (2002).
- ¹³C. Schori, T. Stöferle, H. Moritz, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **93**, 240402 (2004).
- ¹⁴D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).
- ¹⁵M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B **40**, 546 (1989).
- ¹⁶W. Krauth and N. Trivedi, Europhys. Lett. **14**, 627 (1991).
- ¹⁷K. Sheshadri, H. R. Krishnamurthy, R. Pandit, and T. V. Ramakrishnan, Europhys. Lett. **22**, 257 (1993).
- ¹⁸J. K. Freericks and H. Monien, Phys. Rev. B **53**, 2691 (1996); M. Niemeyer, J. K. Freericks, and H. Monien, *ibid.* **60**, 2357 (1999). For recent work in this direction, see P. Buonsante, V. Penna, and A. Vezzani, *ibid.* **70**, 184520 (2004).
- ¹⁹D. Van Oosten, P. van der Straten, and H. T. C. Stoof, Phys. Rev. A **63**, 053601 (2001).
- ²⁰T. Stöferle, H. Moritz, C. Schori, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **92**, 130403 (2004).
- ²¹P. B. Blakie and C. W. Clark, J. Phys. B **37**, 1391 (2004).
- ²²B. B. Baizakov, M. Salerno, and B. A. Malomed, in *Nonlinear Waves: Classical and Quantum Aspects*, edited by F. Kh. Abdullaev and V. V. Konotop (Kluwer Academic, Dordrecht, 2004).
- ²³L. Santos, M. A. Baranov, J. I. Cirac, H. U. Everts, H. Fehrmann, and M. Lewenstein, Phys. Rev. Lett. **93**, 030601 (2004).
- ²⁴N. N. Bogoliubov, J. Phys. (Moscow) **11**, 23 (1947).
- ²⁵E. H. Lieb, R. Seiringer, and J. Yngvason, Phys. Rev. Lett. **94**, 080401 (2004).
- ²⁶D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [*Sov. Phys. Usp.* **3**, 320 (1960)].
- ²⁷F. C. Zhang, C. Gros, T. M. Rice, and H. Shiba, Supercond. Sci. Technol. **1**, 36 (1988).
- ²⁸A. N. Das, J. Konior, D. K. Ray, and A. M. Oles, Phys. Rev. B **44**, 7680 (1991).
- ²⁹M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963).
- ³⁰D. Vollhardt, Rev. Mod. Phys. **56**, 99 (1984).
- ³¹P. W. Anderson, P. A. Lee, M. Randeria, T. M. Rice, N. Trivedi, and F. C. Zhang, J. Phys.: Condens. Matter **16**, R755 (2004).
- ³²L. Tonks, Phys. Rev. **50**, 955 (1936).
- ³³D. B. McWhan, A. Menth, J. P. Remeika, W. F. Brinkman, and T. M. Rice, Phys. Rev. B **7**, 1920 (1973).
- ³⁴W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970).
- ³⁵Y. Tokura, Y. Taguchi, Y. Okada, Y. Fujishima, T. Arima, K. Kumagai, and Y. Iye, Phys. Rev. Lett. **70**, 2126 (1993).
- ³⁶R. Ramakumar, K. P. Jain, R. Kumar, and C. C. Chancey, Phys. Rev. B **50**, 10122 (1994).