Global phase diagram of three-dimensional extended Boson Hubbard model – a continuous time Quantum Monte Carlo study

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We present the global phase diagram of the extended boson Hubbard model on a simple cubic lattice by quantum Monte Carlo simulation with worm update algorithm. Four kinds of phases are supported by this model, including superfluid, supersolid, Mott, and charge density wave (CDW) states, which are identified in the phase diagram of chemical potential $\mu$ versus nearest neighbor interaction $V$. By changing the chemical potential, a continuous transition is found from the Mott phase to a superfluid phase without breaking the translational symmetry. For an insulating CDW state, adding particles to it gives rise to a continuous transition to a supersolid phase, while removing particles usually leads to a first-order one to either supersolid or superfluid phase. By tuning the nearest neighbor interaction, one can realize the transition between two insulating phases, Mott and CDW with the same particle density, which turns out to be of the first-order. We also demonstrate that a supersolid phase with average particle density less than 1/2 can exist in a small region of $\mu - V$ phase diagram.

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I. INTRODUCTION

Lattice models of interacting bosons and fermions such as Hubbard model and its various generalizations are usually strongly correlated systems exhibiting various phases with competing orders, which are of fundamental interest in fields of both condensed matter and cold atomic physics. Interests on both types of Hubbard models are renewed recently, since they can be realized in cold atomic gases loaded in optical lattices (for a review see Refs. 1 and 2 and references therein). Unlike fermions, there is a natural superfluid order for free bosons at zero temperature driven by the kinetic energy. When the interaction is switched on, the bosons are likely to be localized in various crystalline patterns, which may coexist with superfluid order \textsuperscript{3} \textsuperscript{4} to give a realization of intriguing “supersolid” state that has been pursued for decades since 1950s \textsuperscript{5} \textsuperscript{10}. Recently, people have observed the non-classical rotational inertia in solidified \textsuperscript{4}He \textsuperscript{11} \textsuperscript{12} implying a possible supersolid state, which, in spite of the controversy over this topic, also triggers extensive studies on various boson Hubbard models.

Experimentally, the boson Hubbard model can be used to mimic the granular superconductors, where the Cooper pairs are described as bosons, which has been studied by Fisher et al. \textsuperscript{13} two decades ago, where with only on-site repulsive interaction they showed that bosons can form either Mott insulating state with integer filling or superfluid state. Recent experimental progress in cold atomic system provides another realization of boson Hubbard model by loading atoms into an optical lattice with possible long range interactions through dipole interaction \textsuperscript{14} \textsuperscript{16}, or mediated by other intermediate states or fermions \textsuperscript{17} \textsuperscript{19}. In addition, the boson models also share similarities with quantum magnets, e.g., the uniaxial magnetization corresponds to insulating states of boson Hubbard model (e.g. Ref. 20), while the easy-plane magnetization corresponds to the superfluid state. Hence, the studies on the boson Hubbard model may shed light on some common issues of strongly correlated lattice models.

Generally speaking, boson models with interactions at zero temperature have two principal phases: (i) the superfluid and (ii) the incompressible insulating state, which are favored respectively by kinetic and interaction energies, and can coexist. Depending on the features of interaction terms, there are several types of insulating phases, such as Mott, valence bond crystal, and charge density wave (CDW). Note that we in this article define the incompressible states with oscillating density profile as CDW, though the bosons may not carry charges.

The extended boson Hubbard (EBH) model with on-site ($U$) and nearest neighbor ($V$) interactions is a minimal model in favor of CDW and supersolid phases, which has the form of

\begin{equation}
\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i^\dagger) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j - \mu \sum_i \hat{n}_i,
\end{equation}

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where $\hat{b}_i^\dagger$ ($\hat{b}_i$) is the creation (annihilation) bosonic operator at site $i$, $t$ is the hopping amplitude, $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ is the particle number, $\mu$ is the chemical potential, and $\langle i,j \rangle$ runs over all nearest neighbors. Recently, Hamiltonian Eq. 11 and its hard-core version (equivalent to the quantum spin-1/2 XXZ model) with different underlying lattices have been extensively studied in different parameter regimes [5, 6, 21, 28]. However, a global phase diagram of the three-dimensional (3D) EBH model [Eq. 11] is still of lack. As there is no sign problem for the EBH model, the quantum Monte Carlo (QMC) simulation is the most convenient tool for this purpose. The worm algorithm [29, 31] will be invoked to study Hamiltonian 11 on a simple cubic lattice, together with other perturbation and mean-field approaches.

The system described by the EBH model can give rise to a charged ordered crystal at commensurate fillings. The first one is for half filling $\rho = 0.5$, and the corresponding solid state is labeled as CDW I. Doping particles into this state can lead to a supersolid state [5, 6]. However, as shown in Ref. [5], doping holes into it acts quite differently, which may not result in a supersolid state with $\rho < 0.5$, but a phase separation between superfluid and CDW I states, which signals a first-order phase transition. Their argument is based upon the following two observations. (I) Taking one particle out of a perfect CDW crystal with half filling costs almost no potential energy, but only chemical potential. At the same time, the hopping hole also gains a kinetic energy which is quadratic in $t$ ($\sim t^2$). For a perfect CDW crystal, these three processes are balanced, so one cannot take one particle out. (II) The CDW phase breaks the translational symmetry, leading to a two-fold degenerate ground state. If holes are doped into the domain wall between these two degenerate phases, the kinetic energy gained is proportional to $t$. Hence, the CDW phase is unstable toward the domain wall formation if the hole density exceeds $L^{-1}$ for $L^d$ lattice, though it is still stable against losing one particle. This argument perfectly explains the first-order phase transition from the CDW I to superfluid state with $\rho \leq 0.5$, but it fails in two circumstances. The first is that in one dimension the kinetic energy is always linear in $t$, and the corresponding transition is of the Kosterlitz-Thouless type [6]. The other is that if $V$ is comparable to $t$ the kinetic energy of holes is also linear in $t$, which may result in the supersolid phase with the particle density less than half filling (see Sec. III.B). This can be verified by the mean-field calculations [26, 32].

At unitary filling, the ground state can be either a uniform Mott insulator with one particle per site or a charge ordered crystal with two particles on one sublattice and empty on the other one which is labeled as CDW II. There is a critical region around $U \sim zV$, where the two states with different translation symmetries become degenerate, and however, they are separated thermodynamically, i.e., any local perturbation cannot take one to the other. Correspondingly, the transition between them is a first-order one. It is noted that the aforementioned transition from the superfluid to CDW I state by tuning the chemical potential is of the weak first-order [21]. Far less attention has been paid to the region with $zV \sim U$ by now, of which the details are given as part of the phase diagram in this article. To plot the ground state phase diagram, we focus on the case with small hopping and average particle density around or smaller than 1. For larger $t$ or $\rho$, we expect no essentially new physics.

This article is organized as follows. In Sec. III we shall present the global phase diagram. The details of the order parameters will be discussed in Sec. III. The conclusion will be given in last section.

II. GLOBAL PHASE DIAGRAM

A. Classical case with $t = 0$

We start from the classical case without hopping. The energy per site of ground state is a function of the particle numbers on the two sublattices, $n_A$ and $n_B$,

$$\epsilon^{(0)}(n_A, n_B) = -\frac{\mu}{2}(n_A + n_B) + \frac{zV}{2}n_A n_B + U \left[ \frac{1}{2}(n_A(n_A - 1) + n_B(n_B - 1)) \right], \quad (2)$$

where the coordination number $z = 6$ for the simple cubic lattice. The states can be labeled by $(n_A, n_B)$. The Mott states correspond to $n_A = n_B$, and the CDW states with $n_A \neq n_B$ break the translational symmetry, which is two-fold degenerate. In this article, we define the state $(1, 0)$ as CDW I state, and $(2, 0)$ as CDW II state and we only consider $n_A > n_B$ for the CDW states for convenience.

![FIG. 1: (Color online) The phase diagram with zero hopping $t = 0$, where the states are labeled by the particle numbers on two sublattices $(n_A, n_B)$ with the assumption $n_A \geq n_B$. The states with $n_A < n_B$ can be obtained by inversion. The CDW states with one sublattice empty on the right side. Some states can only exist on the green thick solid line, e.g., the states $(3, 1)$ and $(1, 3)$.](image)

For $\mu < 0$ the ground state is a vacuum without any particles. As the chemical potential is increased ($\mu > 0$), the particles are loaded into one sublattice to form a
charge ordered pattern with \( n_A = 1 \) and \( n_B = 0 \), i.e., CDW I state. If we further increase the chemical potential, more particles are loaded into the cubic lattice, which fill either the empty sites if \( zV/U < 1 \) to form a uniform Mott state, or the occupied sites if \( zV/U > 1 \) leading to a CDW II state. In the Mott state, each particle interacts with its nearest neighbors, which effectively lowers the chemical potential to be \( \mu = zV \), and then the critical line between CDW I and Mott states is simply \( \mu = zV \). While that between CDW I and II states is a horizontal line \( \mu = U \) because the chemical potential only needs to compensate the on-site interaction \( U \) for adding new particles.

Similarly, by studying the instability of adding particle to a state \( (n_A, n_B) \), one can determine all the phase boundaries between different classical insulating states, as shown in Fig. 1. There is a special vertical line \( zV/U = 1 \), on which many states can coexist with the same free energy. For example, on the boundary between Mott and CDW II states, there are actually three macroscopic states, which are \((1,1)\), \((2,0)\) and \((0,2)\). In fact, some of them only exist on this line in the absence of hopping terms, e.g., states \((3,1)\) and \((1,3)\) on the boundary between Mott \((2,2)\) and CDW \((4,0)\) states. These degenerate states are macroscopic which cannot be transformed to each other smoothly by local perturbations, i.e., there are infinitely high barriers between these macroscopic states.

**B. Case for finite \( t \)**

For the case with a finite hopping \( t \), the particles (holes) adding to an insulating state can gain a kinetic energy, which results in the shrinking of insulating areas in the phase diagram (Fig. 2) comparing with the classical case (Fig. 1). In three dimensions, these mobile bosons condense at low temperature leading to the superfluidity, which enriches the phase diagram. There are four phases for the EBH model characterized by the following three quantities: the particle density \( \rho \), superfluid density \( \rho_s \), and static structure factor \( S_\pi \) at momentum \( \vec{\pi} = (\pi, \pi, \pi) \) with

\[
\rho_s = (W_x^2 + W_y^2 + W_z^2)/(2\beta m),
\]

\[
S_\pi = \frac{1}{N^2} \sum_{\vec{r}, \vec{r}'} e^{-i\vec{\pi} \cdot (\vec{r} - \vec{r}'')} \langle n_{\vec{r}} n_{\vec{r}'} \rangle,
\]

where \( W_{x,y,z} \) are the winding numbers along \( x, y \) and \( z \) directions, \( \beta \) is the inverse temperature, and \( m = 2/t \) is the effective mass of the bosons. In the insulating Mott and CDW states, particles are localized by the interaction and the local particle number is quantized as in the classical case. The pure superfluid state has nonzero superfluid density \( \rho_s \) and a vanishing static structure factor \( S_\pi \), while both are finite in the supersolid phase.

Fig. 2 is the phase diagram determined by the QMC simulation with the worm update algorithm, where the solid lines with circles are the QMC results and the dotted lines are from the perturbation expansion in the strong coupling limit \( z < 1 \) where the insulating states become unstable against adding or removing particles. It is seen that the perturbation results agree quite well with those of the QMC simulation in part of the phase diagram, but it is still not applicable in some regions since it cannot deal with the superfluid order.

Comparing with the classical case in Fig. 1 the CDW I state is detached from its insulating neighbors, i.e., the Mott, CDW II and vacuum states. The upper boundary of vacuum state is actually lowered below \( \mu = 0 \) due to the hopping of bosons, which is not shown in Fig. 1. The gaps between different insulating states are filled with the superfluid and supersolid phases. The lower boundary of CDW I state is a critical line on which there occurs a phase separation between the superfluid and CDW I phases, which breaks the U(1) gauge symmetry and the translational symmetry, respectively. The transition between them is of the weak first-order across which the particle density and superfluid density have a jump. Considering the correspondence between the EBH model and spin models, this transition is similar to the spin-flopping process in the two- or three-dimensional anisotropic XXZ model in the presence of magnetic field pointing in \( z \)-axis, which is equivalent to the EBH model in the hard-core limit \( [33, 35] \). As explained in Ref. [5], this first-order
phase transition with a particle number jump is due to the fact that the CDW I phase is unstable toward the domain wall formation if the filling number exceeds $L^{-1}$ though it is still stable against doping one hole. Doping particles upon the CDW I phase by increasing the chemical potential does not lead to a first-order transition as in the hard-core EBH model (or equivalently the XXZ model), where the particle-hole symmetry makes the upper and lower boundaries of CDW I phase identical. In case of the soft-core bosons, these additional particles can move upon the alternating charge ordered background with the effective hopping amplitude $t^2$, which can Bose condense at zero temperature without destroying the staggered density order, and thus leads to a supersolid state with $\rho > 0.5$. This transition is of a second-order, as shown by a green solid line in Fig. 2 where all the second-order phase boundaries are in green that are distinct from the first-order ones which are colored in red.

Continuously increasing the chemical potential upon supersolid phase, two different situations occur. (1) For $zV < U$, the particles like to occupy the empty sites which weakens the CDW order accompanied by the occurrence of superfluid order. Until some critical filling $\rho < 1$, the CDW order is completely destroyed and a pure superfluid state appears with the translational symmetry restored. The transition is of the second-order. (2) For $zV > U$, the additional particles are added to the occupied sites so that the CDW order is actually enhanced until finally entering into another insulating state, CDW II, through a first-order phase transition, of which the reason is the same as that from the superfluid with $\rho < 0.5$ to CDW I. In this sense, the staggered density order in supersolid phase is inherited from the CDW I state, not related to the CDW II state, since doping holes to the CDW II state cannot smoothly result in the supersolid state.

As shown in the previous study [3], doping holes into the CDW I state may not lead to supersolid state with $\rho < 0.5$ on a two-dimensional square lattice, contrary to the case of doping particles. The reason is that the CDW I state has two-fold degeneracy. As long as enough particles are removed, the insulating state becomes unstable towards the formation of domain walls between the two degenerate states, but can still be stable against losing one particle. This explains the particle density jump across the first-order phase boundary between the superfluid and CDW I phases and that between the supersolid and CDW II phases. However this argument is invalid for $V$ close to $t$ that is around the tip of the CDW I lobe, where we show below that the kinetic energy gain by doping one hole into the CDW I state is also linear in $t$, that can cause instability of CDW I state towards a supersolid state without the formation of domain walls. Suppose that one particle is taken from a CDW I state, the hole leaving behind moves in an effective staggered potential, roughly speaking, 0 in one sublattice and $(z-2)V$ in the other. Solving this single particle problem, one estimates the kinetic energy gain $\Delta K$ is

$$\Delta K = -t^2 \left[ \frac{V}{2t} (1 - \frac{2}{z}) + \sqrt{1 + \left( \frac{V}{2t} \right)^2 (1 - \frac{2}{z})^2} \right]^{-1}$$

which is about $-2.88t$ in the cubic lattice near the tip of CDW I lobe where $V \sim 2.4t$ (see Fig. 2). As a consequence, a supersolid phase with $\rho < 0.5$ occurs, whose boundary is plotted in the inset of Fig. 2. To confirm, we also extrapolate the static structural factor, superfluid order and particle density at point $zV = 0.3635U$ and $\mu = 0.145$ to the thermodynamic limit (see Fig. 3), which indicates a supersolid state with the particle density less than half filling. For more information, one can refer to next section where we shall examine the order parameters in details.

In the presence of a kinetic term, the vertical boundary at $zV \sim U$ between Mott and CDW II states does not yet split but moves slightly to the CDW side. On this boundary, the free energies of both states are equal. However, they have different symmetries and are separated from each other thermodynamically. The transition between these two insulating states is of the first-order, which is similar to the conventional liquid-solid phase transition. Further doping particles into the Mott and CDW II states leads to the reentrance of superfluid and supersolid states, respectively, with density $\rho > 1$.

Because the particles or holes can hop between nearest neighbors on a Mott background, which leads to a kinetic energy gain linear in $t$, however they can only hop among next nearest neighbors in a staggered CDW background that gives rise to a hopping energy proportional to $t^2/V$. Then, as $t$ increases the Mott region shrinks much faster than the CDW II region, which results in the mismatch of phase boundary between them as $zV \sim U$(see Fig. 2). Since doping the Mott state with holes leads to a superfluid state, one expects a boundary between the superfluid state and the CDW II state in the critical region at the lower end of the vertical boundary.

![Figure 3](image_url)

**FIG. 3:** (Color online) The extrapolation of the order parameters in the supersolid phase with $\rho < 0.5$. In the thermodynamic limit, the staggered structure factor $S_x = 0.14$, the superfluid density $\rho_s = 0.17$ and the particle density $\rho = 0.496$, which indicates a supersolid state less than the half filling.
This phase boundary is again of the first-order. At the upper end, the extension of the vertical boundary separates the superfluid and supersolid phases in the way of the second-order phase transition.

III. ORDER PARAMETERS

![FIG. 4: (Color online) The average particle density \( \rho \) as a function of chemical potential \( \mu \) for different \( V \) and \( U = 40t \). The first plateau at \( \rho = 0.5 \) corresponds to the CDW I phase, and the second one corresponds to the Mott phase for \( V/t = 3, 4, 5 \) and the CDW II phase for \( V/t = 9 \). The system size is \( 12 \times 12 \times 12 \).](image1)

In this section we give the details of the parameters \( \rho, \rho_s \), and \( S_\pi \) for different \( \mu \) and \( V \). Fig. 4 is the density profile as we vary the chemical potential for several fixed values of \( V \), where the plateaus correspond to the incompressible states, i.e., the Mott, CDW I and II states, with vanishing isothermal compressibility \( \kappa_T \equiv \rho^{-2} \partial \rho / \partial \mu \). Note that these insulating states correspond to two single points \( \rho = 0.5 \) and \( \rho = 1 \) in Fig. 4 which is the plot of superfluid density \( \rho_s \) and \( S_\pi \) as functions of particle density \( \rho \).

For \( \rho < 0.5 \), the particles Bose condense to form a pure superfluid state with a nonzero \( \rho_s \) but vanishing \( S_\pi \) as shown in Fig. 5. When the particle density reaches a commensurate value \( \rho = 0.5 \), a plateau appears implying \( \kappa_T = 0 \) which corresponds to the incompressible CDW I state with translational invariance broken. This transition is of the first-order since the particle density, as a first-order derivative of free energy with respect to the chemical potential, is discontinuous. This is also reflected in Fig. 5 as the fact that a segment of particle density \( \rho_s \) and \( S_\pi \) jumps at \( \rho = 0.5 \) to a finite value from zero. As the particle density exceeds 0.5, \( \kappa_T \) becomes a finite positive value again. At the same time the superfluidity appears continuously upon the CDW I state to form a supersolid. The corresponding transition is of the second-order, since the particle density \( \rho \) is continuous but \( \kappa_T \) jumps from zero to a finite value.

Between the two plateaus at \( \rho = 0.5 \) and \( \rho = 1 \), the slope of \( \rho(\mu) \) curve for \( V/t = 3, 4 \) and 5, i.e. \( zV < U \), shows another jump, implying that \( \kappa_T \) is discontinuous and a second-order phase transition from the superfluid to superfluid phase occurs. This transition is manifested in Fig. 5 where \( \rho_s \) keeps finite in the whose region \( 0.5 < \rho < 1.0 \), but \( S_\pi \) vanishes at some critical values in between. Further increasing the chemical potential, the system enters into the Mott phase, which corresponds to the plateau with \( \rho = 1 \) in Fig. 4 through a second-order phase transition. At the transition point \( \rho_s \) vanishes as shown in Fig. 5.

For \( V = 9t \), i.e., \( zV/U > 1 \), the second plateaus in Fig. 4 corresponds to the CDW II state, into which the system enters directly from the supersolid phase as \( \mu \) is increased. The transition is a first-order one as shown in Fig. 4 as the jump of particle density. It is also reflected in Fig. 5 where a segment of particle density \( \rho \) is not accessible before \( \rho \) reaches 1.

In Fig. 5, we plot the normalized order parameters \( \rho_s \equiv \rho_s / \rho_{s,max} \) and \( S_\pi \equiv S_\pi / S_{\pi,max} \) as functions of \( zV/U \) around the CDW I lobe, where \( \rho_{s,max} \approx 0.6 \) and \( S_{\pi,max} \approx 0.2 \). In the plot, we take three characteristic values of the chemical potential \( \mu/U = 0.160, 0.155 \) and 0.145 from the top to the bottom panel. In the shaded areas, when \( V \) increases, the superfluid density \( \rho_s \) decreases while the static structure factor \( S_\pi \) increases, and both \( \rho_s \) and \( S_\pi \) are nonzero in this region indicating a supersolid state. The supersolid area becomes more and more narrow as \( \mu \) decreases, until finally shrinks to a point in the \( zV/U \) axis when \( \mu/U \sim 0.140 \), which implies that two second-order phase boundaries merge into one first-order phase boundary across which the order parameters \( \rho_s \) and \( S_\pi \) are both discontinuous. The corresponding density profiles are plotted in Fig. 5, where we observe that the particle density is always smaller than 0.5 for \( \mu/U = 0.145 \) corresponding to the bottom panel in Fig. 5 until it enters into the CDW I phase, that implies the supersolid state can exist below the half filling. For \( \mu/U = 0.160 \), the situation is different where
ρ decreases as V is increasing, which can be intuitively attributed to the loss of effective chemical potential due to nearest neighbor interaction V in the mean-field level. The case of μ/U = 0.155 shows an intermediate behavior, for which the particle number first decreases, then increases slightly larger than 0.5 and finally reaches the CDW I state.

In this article, we present the global phase diagram (Fig. 2) of the 3D extended Bose Hubbard model. The EBH model exhibits four kinds of ground states, including (1) the Mott state without breaking any symmetry, (2) the CDW I and II states with translational symmetry broken, (3) the superfluid with U(1) gauge symmetry broken, and (4) the supersolid with both symmetries broken. By using the QMC simulation as well as other analytical tools, we identify the transition type between these phases. Among them, the first-order phase boundary includes those between the superfluid and CDW (I and II) states, and between the Mott and CDW II states. The other boundaries are all continuous. The critical regions for zV/U ∼ 1 and the tip of the CDW I lobe are examined in detail. We demonstrate that in the present 3D EBH model, the supersolid phase with ρ < 0.5 can appear in a small region near the CDW I lobe where the hopping amplitude t is comparable to the nearest neighbor interaction V. In this region, the general “domain wall” argument for the nonexistence of supersolid state with ρ < 0.5 is no longer applicable, since it is based on the assumption of t ≪ V.

V. ACKNOWLEDGMENT

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