Frustration induced incommensurate solids in the extended Bose-Hubbard model

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We study the extended Bose-Hubbard model with nearest-neighbor and next-nearest-neighbor \((V, V')\) repulsive interactions on a square lattice by using the quantum Monte Carlo method. Unlike the case of strong \(V'\) where the ground states can be striped solids or striped supersolids, we focus on weak \(V' < V/2\) and small hoppings and find that, in the thermodynamic limit, incommensurate solids of fractional densities varying from 1/4 to 1/2 can be stabilized. We also show that the incommensurate solids, which are characterized by a continuous set of wave vectors changing from \((\pi, \pi/2)\) (or \((\pi/2, \pi)\)) to \((\pi, \pi)\), can be understood by a mechanism of domain wall formation. The related ground-state phase diagram and thermal phase transitions are also discussed.

I. INTRODUCTION

Polar molecules trapped in optical lattices provide an unique opportunity to study the dipole-dipole interactions in real experimental setups \([1,4]\). One primary investigation is to identify possible quantum phases that may uniquely arise from these long-range interactions but cannot be observed in shorter range interactions (like nearest-neighbor (nn) and next-nearest-neighbor (nnn)). Recent numerical studies \([5-8]\) of hard-core \((\text{nn} \text{ and nnn})\) with infinite-range interactions on two dimensional (2D) square lattices have presented evidences of Mott solids with checkerboard, stripe, and star ordering, corresponding to densities \(\rho = 1/2, 1/3, \) and 1/4 respectively. Furthermore, supersolids around the Mott lobes with \(\rho = 1/2\) and 1/4 are also found by doping the solids with particles or vacancies. Besides the above mentioned densities, density plateaus of other rational fillings that constitute the devil’s staircase is observed, which signals the presence of the incommensurate phases.

Nevertheless, the presence of the Mott solids and supersolids is not unlike the ground-state phases of the short-range models. Previous numerical results on the extended Bose-Hubbard model that includes only the nn and nnn interactions have indeed observed the Mott solids and supersolids of 1/2 and 1/4 fillings \([9-14]\). The Hamiltonian of the hard-core extended Bose-Hubbard model with nn and nnn interactions in 2D square lattices is,

\[
H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h\text{c.}) + V \sum_{\langle i,j \rangle} n_i n_j + V' \sum_{\langle i,j \rangle'} n_i n_j - \mu \sum_i n_i,
\]

where \(b_i \text{ (} b_i^\dagger \text{)}\) is the annihilation (creation) bosonic operator on site \(i\), \(V\) and \(V'\) the nn and nnn interactions respectively and \(\mu\) the chemical potential that controls the particle density in the grand canonical ensemble. Mott solids of striped and star orders at 1/2 and 1/4 filling respectively are observed for small \(V < 2V'\), both associated with supersolids of the same orderings. Therefore the presence of these phases in this short-range model suggests that the long-range nature of the dipole-dipole interactions is not indispensable to the stability of these phases.

One may still wonder, however, if the incommensurate phase indicated by the observed devil’s staircase is a unique consequence of long-range interactions on the square lattice, or are shorter range interactions sufficient to stabilize the incommensurate solids just as the case in the geometrical frustrated triangular lattice \([15, 16]\). In addition, the nature and stability of such an incommensurate phase are of great interest on its own, and the understanding of which should shed light on the other frustrated systems. However, it is hard to address these fundamental issues in the infinite-range model.

In this work, we employ the quantum Monte Carlo (QMC) method with stochastic series expansion algorithm \([17, 18]\) in a short-range model to show that at small hopping \(t\) and strong nn interactions \(V\), incommensurate solids of densities range from 1/4 to 1/2 can be also stabilized in the thermodynamic limit. The ground-state phase diagram as one of our main results is presented in Fig. 1, where incommensurate solids emerge between the half-filled checkerboard and quarterfilled solids. In contrast to the weak-\(V\) cases \([9, 13]\), there exists no super-solid phases in the present case of \(V > 2V'\). We find that the incommensurate solids exhibited in the ground-state phase diagram are characterized by continuously changing wave vectors as systems parameters are changed. The formation of such a phase can be explained by the insertion of domain walls into half-filled or quarter-filled solids. Following the analysis in the anisotropic triangular lattice \([16]\), an analytical model of the domain-wall excitations on our square lattice system is proposed and its predictions do agree very well to the QMC numerical results. Furthermore, the quantum phase transitions from the incommensurate solids to the half-filled or quarter-filled solids are found to be continuous in the thermodynamic limit, while the transition to the superfluid phase is first-order. Upon increasing temperatures, the incommensurate solids will melt into normal fluids via a first-
order thermal phase transition, which are demonstrated by hysteresis of the structure factors and double peaks in histogram.

II. QUANTUM PHASE DIAGRAM

In this work we utilized the well established stochastic series expansion algorithm [17,18] in the QMC calculations as the Hamiltonian $H$ in Eq. 1 is sign-problem free. We set $V' = 1$ (unless mentioned otherwise) as the energy scale and the inverse temperature $\beta = 1/2L$, where $L$ is the lattice size ($L=12, 24, 36, \text{and} 48$ are used). To identify various phases, we measured in our simulation the superfluidity $\rho_s$ that signals off-diagonal U(1) symmetry breaking, and is defined by the fluctuations of winding number that

$$\rho_s = \frac{1}{2\beta} (\langle W_x^2 \rangle + \langle W_y^2 \rangle). \quad (2)$$

On the other hand, the translational broken symmetry is characterized by the structure factor

$$S(Q) = \frac{1}{L^2} \sum_{i,j} \langle n_i n_j \rangle e^{iQ \cdot r_{ij}}, \quad (3)$$

where the wave vector $Q$ defines the solid ordering.

In the parameter regime we studied in our model, the off-diagonal and diagonal ordering do not coexist, that means no supersolid (SS) is found. In Fig. 1 the ground-state phase diagram $\mu$ vs $t$ with $V = 4$ contains solid states of definite wave vectors and a superfluid (SF). The phase boundaries are determined by the abrupt changes of $\rho_s$ or $S(Q)$ (see Fig. 2) and by extrapolating to the thermodynamic limit with $L \rightarrow \infty$. At the limit of zero hopping $t = 0$, the half-filled phase is a checkerboard solid (CBS) with $Q = (\pi, \pi)$, instead of a striped solid, because the nn repulsion is dominant ($V > 2V'$) so that nn occupation is avoided. Reducing the chemical potential to $\mu < 4$, the ground state is then a quarter-filled solid (QFS) of star ordering [12,13] with $Q = (\pi/2, \pi)$ or $(\pi, \pi/2)$. While there are two types of star orders that are doubly degenerate at $t = 0$, the degeneracy is lifted for finite $t$. The QFS ordering shown in the inset of Fig. 1 is favorable as it prevents nn occupation up to second order of hopping $t$ to reduce the cost of nn potential energy. Interestingly, for finite but small $t$, the phase in between the CBS and QFS is not a superfluid or supersolid, but a series of incommensurate solids (ICS) with wave vectors $Q$ continuously varying from $(\pi/2, \pi)$ or $(\pi/2, \pi)$, to $(\pi, \pi)$ in the thermodynamic limit. We found that ICS can be understood by inserting the domain walls into the solid phases. We will discuss the nature of the ICS in the next section. For even larger hopping, all solid phases eventually melt into a superfluid phase directly without passing an intermediate supersolid phase. Further discussions on the phase transitions will be provided in section V.

III. INCOMMENSURATE SOLIDS

By fixing the hopping $t = 0.4$, the particle density $\rho$ is shown in Fig. 3 for $L = 36$. A series of density plateaus

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FIG. 1. Ground-state phase diagram $\mu$ vs $t$ with $V = 4$ obtained from QMC calculations that extrapolated to thermodynamic limit. The dotted lines are the phase boundaries predicted by the domain wall analysis. The insets show the CBS and the QFS lattice structure.

FIG. 2. Order parameters vs $\mu$ with $t = 0.4$ and $V = 4$. Lattice size $L = 36$. Upper panel: the particle density $\rho$ as a function of $\mu$. The fractional numbers are the corresponding densities of the plateaus. Open circles are the density for $L = 24$. Lower panel: superfluidity $\rho_s$ (filled squares) and structure factors $S(Q)$ (open circles) as a function of $\mu$. The corresponding wave numbers of the data are, from left to right, $Q = (\frac{2m}{L} \pi, \pi)$ with $m = \frac{L}{4} + 1, ... , \frac{L}{2}$. (note that the data of $S(\pi, \pi)$ is reduced by 5 times.)
is observed from \( \rho = 1/4 \) to \( 1/2 \), in between of the QFS and CBS. It is noted that the plateaus occur at densities of \( m/L \), with \( m \) an integer from \( L/4 \) to \( L/2 \). This is very similar to the staircase found in the model with infinite-range interactions [3, 5]. In that case, although a smaller lattice size \( (L = 12) \) is used, much more plateaus of rational fillings are found between density \( \rho = 1/4 \) and \( 1/2 \). The reason for this discrepancy is that the infinite-range nature of the interactions allows more possible configurations of particle ordering to be stabilized, which, unfortunately, also makes it more difficult to analyze the properties of the ICS. Contrarily, in our model, we can understand the origin of the density plateaus with a simple picture of linear fluctuating domain walls.

By doping the half-filled CBS with holes, the potential energy gain is \( 4V' \) for each addition isolated hole. Nevertheless, holes that aligned together to form a domain wall (Fig. 3(b)) can further gain kinetic energy through particle hoppings, which will be explained in detail in the next section when we discuss the domain wall dynamics. To facilitate discussion, we define \( L_x \) (\( L_y \)) be the lattice size in the \( x \) (\( y \)) direction. It is noted that even number of domain walls is required to maintain the periodic boundary condition imposed in our system. Consequently, doping the holes in the CBS resulted in removing \( L_y/2 \) particles (assume the domain walls extend along the \( y \) direction) for each domain wall, and totally \( nL_y/2 \) particles for \( n \) domain walls in the lattice, where \( n=0, 2, 4, ..., L_x/2 \). When there are \( L_x/2 \) domain walls, it corresponds to the quarter-filled solid state (Fig. 3(d)). Therefore, the particle density \( \rho \) is expected to be \( (L_x - n)/2L_x \) in the domain wall states, which exactly corresponds to the density of the plateaus found in Fig. 2 for both \( L = 24 \) and \( 36 \) (note that \( L = L_x = L_y \) in all simulations). Furthermore, the presence of domain walls is also evident by the shift of structure factor peaks. It is noted that the addition of domain walls does not completely destroy the checkerboard order \( (Q=(\pi, \pi)) \), but shifts the peak of the structure factor by \( (\pi/L_x, 0) \) for each added domain wall. Hence the plateau states in ICS can be characterized by the wave vectors \( (\pi - n\pi/L_x, \pi) \) or \( (2m\pi/L_x, \pi) \) with \( m \) an integer from \( L_x/4 \) to \( L_x/2 \). This is consistent to the numerical result shown in Fig 2.

Another implication from the above analysis is that as \( L \to \infty \), the number of plateaus will become infinity such that \( \rho \) changes continuously from \( 1/4 \) to \( 1/2 \). The jump at the phase boundary between QFS (CBS) and ICS is then expected to be reduced to zero, which implies the commensurate-incommensurate transition is continuous. The location of these phase boundaries in the ground-state phase diagram for small \( t \) can be determined analytically by considering the domain wall dynamics, as will be discussed in the following section.

### IV. DOMAIN WALL DYNAMICS

The analysis of domain wall dynamics can be borrowed from the result of anisotropic triangular lattice [16], in which system incommensurate supersolids are found. Started with the half-filled CBS state, by doping of holes we add a column of vacancy in the checkerboard ordering as depicted in Fig. 3(a) that splits the CBS into half. Shifting half of the lattice does not cost any addition potential energy, but the bosons on the shifted boundary are now free to move sideways such that the domain wall boundary can fluctuate to gain the kinetic energy. Specifically we define the domain walls by connecting the center of unoccupied bonds, the red zigzag chain in Fig. 3(b). As illustrated in the figure, after the hopping of bosons, part of the resulted domain wall, dotted lines, fluctuates in the direction of the particle movement. To estimate the domain wall energy, one can map the one-dimensional (1D) domain wall into a 1D spin-1/2 XY chain [10, 19, 20]. By tracing the zigzag chain along \( y \) direction, if the \( x \)-coordinate is increased (decreased) by one unit, a up (down) spin is assigned to the corresponding bond. The kinetic energy of a domain wall is then corresponding to the spin flip of the 1D spin chain, whose kinetic energy per unit length has been shown to be \( \Delta E_k/L_y = -2t/\pi \) [19]. While the change in potential energy per unit length of inserting a domain wall (removing \( L_y/2 \) bosons) is \( \Delta E_p/L_y = (\mu - 4V')/2 \), the critical \( \mu_c \) can be derived from \( \Delta E = 0 = (\mu_c - 4V')/2 - 2t/\pi \), i.e.

\[
\mu_c = 4V' + \frac{4t}{\pi}.
\]
This quantum phase boundary is plotted in Fig. 1 (dotted lines), which is in good agreement with the QMC result.

For the transition from QFS to ICS, the same argument applies. Doping the QFS with a column of bosons, it actually generates two domain walls. Here we define the domain wall as the line connecting nn bosons. Again, by mapping the domain walls to 1D spin-1/2 chain, the kinetic energy per unit length is equal to 2\(\times (2t/\pi)\). With the potential energy change per unit length equals to \((4V' - \mu)/2\), the critical \(\mu_{c2}\) is given by:

\[
\mu_{c2} = 4V' - \frac{8t}{\pi},
\]

which is again in good agreement with the numerical result. Derivations are expected for large \(t\) when higher order corrections and SF fluctuations are important.

Following the analysis by Zhang et al. [16] in anisotropic triangular lattice, we also determine the domain wall density \(\rho_D\) as a function of \(\mu\). In the QMC calculation, \(\rho_D\) is defined as:

\[
\rho_D = \frac{1}{L_x L_y} \sum_{x,y} \tilde{n}_{x,y} \tilde{n}_{x+1,y},
\]

where \(\tilde{n}_{x,y} = 1 - n_{x,y}\) is the hole number (0 or 1) at site \((x,y)\). Here \(\tilde{n}_{x,y} \tilde{n}_{x+1,y}\) counts the number of hole-hole bonds in the \(x\) direction. The QMC result of \(\rho_D\) is shown in Fig. 4.

Clearly, the domain walls will interact with each other with an energy \(f(\rho_D)\) that depends on the density \(\rho_D\). This unknown function \(f(\rho_D)\) can be determined by fitting to the numerical results. Now, the total domain wall energy at density \(\rho_D\) is given by

\[
E(\rho_D) = L_x L_y V' \rho_D \left[ -2 + \frac{\mu}{2V'} - \frac{2t}{\pi V'} + f(\rho_D) \right].
\]

The transition from \(2M - 2\) domain walls to \(2M\) domain walls occurs when \(E(\frac{2M-2}{L_x}) = E(\frac{2M}{L_x})\) which leads to the recursive relation of \(f(2M/L_x)\):

\[
\mu_M = \mu_{c1} + 2V' \left[ (M - 1)f(\frac{2M-2}{L_x}) - Mf(\frac{2M}{L_x}) \right].
\]

This can be solved to have

\[
f(\frac{2M}{L_x}) = \frac{1}{M} \left[ \frac{\mu_{c1}}{2} - \sum_{i=1}^{M} \frac{\mu_i}{2M} \right].
\]

As a result, the simulated values of \(\mu_M\) can be used to evaluate the discrete values of \(f(2M/L_x)\). As shown in the inset of Fig. 4, a power-law function \(A\rho_D^\alpha\) can be fitted to the \(f(\rho_D)\) with the exponent \(\alpha = 3.4(2)\) for \(t = 0.4\) (upper panel). With this result, the domain wall energy of Eq. 2 is then minimized to obtain the domain wall density

\[
\rho_D = \left[ \frac{\mu_{c1} - \mu}{2V' A(\alpha + 1)} \right]^{1/\alpha}.
\]

This result is found in good agreement with the simulated result in Fig. 4 and hence justifies the application of the domain wall dynamic model in our system. Interestingly, we repeated the same domain wall density calculation for \(t = 0.2\) and obtained nearly the same exponent \(\alpha = 3.6(3)\), suggesting possible universal exponent for different hopping integrals.

V. INCOMMENSURATE-SUPERFLUID AND THERMAL PHASE TRANSITIONS

The quantum phase transitions from all solid states, in our parameter regime, to superfluid phase are observed to be discontinuous, without the appearance of immediate supersolid phase. In Fig. 5, it demonstrates the abrupt changes of superfluidity \(\rho_s\) and structure factors across the phase boundary from two plateau states (1/3 filling and 7/24 filling respectively) to SF as the hopping \(t\) is increased. Noticed that the solid ordering is destroyed at the same critical \(t\) where the superfluidity \(\rho_s\) emerges and no signs of coexistence of both order parameters is found. The absence of supersolid phase could be accounted by the same argument for CBS and QFS that phase separation is favorable to the supersolid phase [9]. For the
transitions from the incommensurate solids to CBS or QFS, in the thermodynamic limit where there are infinite number of plateau states, the particle density $\rho$ is expected to be varied continuous from $\frac{1}{3}$ to $\frac{1}{2}$. While the broken symmetry of CBS is different from that of QFS, it is interesting to note that a continuous change of broken symmetry in the ICS connects these two phases via second-order phase transitions.

By increasing $V^\prime$, the enhanced nnn frustrations will reduce the cost of potential energy change per each domain wall (see section IV). Therefore, the system will move down along the density plateaus as larger $V^\prime$ will generate more domain walls of holes. Our numerical result for $V = 4$ at $\mu = 4.0$ and $\mu = 4.6$ plotted in Fig. 6 are consistent with this prediction. At $\mu = 4.0$, the system moves from the $\frac{1}{4}$-filling state all the way to the quarter-filling state as $V^\prime$ increases. However, at $\mu = 4.6$, for $V^\prime > 1.24$ the frustration is too strong that diagonal long-range order cannot be sustained and the system melts into a superfluid phase instead. An abrupt jump of superfluidity is observed that signals a direct first-order phase transition from ICS to SF, without an intermediate supersolid phase.

We also study the thermal phase transitions of the ICS phase and QFS phase. The broken translation symmetry of the ICS and QFS is restored by thermal fluctuations at high temperature, which can be identified by the disappearance of the corresponding structure factors. A careful study of the order-disorder transitions indicate that the transitions are of first order. In Fig. 7 we measure the structure factors $S(2\pi/3, \pi)$ and $S(\pi/2, \pi)$ of the $\rho = 1/3$ ICS phase and $\rho = 1/4$ QFS phase respectively. At the first glance, the thermal transitions seem to be continuous, but a detail analysis shows the typical hysteresis behavior of discontinuous phase transitions around the transition temperatures. Starting from the order (disorder) states, we increase (decrease) the temperature slowly in the QMC simulation using the operator lists taken from previous temperature as initial conditions. From Fig. 7 it is clearly that results from increasing and decreasing temperature follow different paths around the phase transitions. Double peaks are also observed in the histograms (insets in Fig. 7) which confirmed the nature of first-order transition. It is noted that previous study of another type of quarter-filled solid suggested a continuous thermal phase transition [14]. This difference can be explained by the dis-

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**FIG. 5.** Phase transition from ICS to SF states for (a) $\mu = 4.0$ and (b) $\mu = 3.2$ as a function of $t$, for $V = 4$ and $L = 24$. Both superfluidity $\rho_s$ (open circles) and structure factor $S(Q)/N$ (open squares) show signature of first-order phase transition from ICS to SF states.

**FIG. 6.** The boson density $\rho$ (circles) and superfluidity $\rho_s$ (squares) as a function of $V^\prime$ with $V = 4$ for (a) $\mu = 4.0$ and (b) $\mu = 4.6$, with $L = 36$ and $V = 4$.

**FIG. 7.** Hysteresis of the structure factors $S(Q)$ at (a) the $1/3$-filling plateau state ($\mu = 4.0$), and (b) the $1/4$-filling QFS state ($\mu = 2.0$). The insets show that the double peaks feature of $S(Q)$ around the transitions. Lattice size $L = 24$ and $V = 4$. 
tinct broken symmetries of these two types quarter-filled solids. Furthermore, it is noticeable that the hysteresis loop becomes much smaller and the double peaks feature less significant in the ICS than the case of the QFS. This indicates that, as the chemical potential $\mu$ increases from the QFS to ICS, the first-order thermal phase transition becomes weaker. This is consistent to the fact that the thermal transition of half-filled CBS is known to be continuous, so that approaching the CBS from 1/4-filled QFS via 1/3-filled ICS, the thermal transition is expected to evolve from strong first-order to weakly first-order and then to second-order. Since the wave vector $Q$ of maximum structure factor varies continuously in the ICS phase into the CBS, it is natural to expect a smooth evolution of transition order instead of an abrupt change as $Q$ approaches to $(\pi, \pi)$.

VI. CONCLUSION

We have shown that the incommensurate solid states can emerge in a square lattice even with shorter range of frustrated interactions, which has been overlooked in previous studies of extended Bose-Hubbard model. The ICS phase appears in between the half-filled solid and quarter-filled solid and is characterized by density plateaus of fractional values. The shorter range of interactions in our model simplifies the analysis and allows us to address fundamental questions about the nature of the plateau states. In our model, we propose a domain wall theory that accounts for the fractional values of particle densities and the peaks of the structure factors of the plateau states. Furthermore the measured domain wall densities $\rho_D$ agree well with the predicted values from the theory of the interacting domain walls, in which the interaction term behaves as a power-law function of $\rho_D$ with an exponential being independent of the hopping integrals. In the thermodynamic limit we expect the wave vector $Q$ characterizing different broken symmetries changes continuously from $Q = (\pi/2, \pi)$ for the quarter-filled star order to $Q = (\pi, \pi)$ for the checkerboard order with the widths of the intermediate plateau states diminished. There is no superfluidity found in the ICS phase, differs from the case of anisotropic triangular lattice where an incommensurate supersolid is observed. It is not surprising as in the triangular lattice, bosons have more degrees of freedom to hop around than the counterparts in the square lattice. Based on this observation, one may expect incommensurate supersolids to survive if nnn hopping is turned on in our model. It is also interesting to consider the effect of strong frustration (large $V'$) on the ICS phase. We show that stronger $V'$ can melt the ICS phase or push the system to become a QFS. However, it is known that for even larger $V'$ another type of star order is favorable at quarter filling, whether similar ICS phase can be induced is not clear without extensive studies on a wide range of parameter regime. Furthermore, while we have shown that nnn frustration is sufficient to induce the ICS phase in a square lattice, how does the domain wall mechanism evolve to generate the staircase observed in the case of infinite range interactions will also be worth to investigate in a further study.

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