Effects of frustration on the anisotropic triangular lattice bosons

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We study the extended hard-core Bose-Hubbard model with nearest-neighbor interactions on a triangular lattice with spatial anisotropy by quantum Monte Carlo simulations. The effects of the geometric frustration or the anisotropic strength, represented by the ratio t'/t between the intrachain nearest-neighbor hopping t' and the interchain hopping t, are studied. We find that for small values of anisotropy ratio t'/t, a solid state emerges at $\rho=1/2$ and a supersolid is unstable toward phase separation; for large values of anisotropy ratio t'/t, solid states emerge at $\rho=1/3$, 2/3, and a supersolid phase is stable in the region $\rho<2/3$; for intermediate values of anisotropy ratio t'/t, three kinds of solid states at fillings $\rho=1/3$, 1/2, and $\rho=2/3$ coexist and no stable supersolid phase is observed. At half filling, we find that with increasing frustration t'/t, the $\rho=1/2$ solid transitions indirectly into the supersolid via an intervening superfluid.

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I. INTRODUCTION

In the past several years, the Bose-Hubbard model and its extensions have been extensively studied on various lattices.[1–18] This is partially due to the potential realization of these models in ultracold atoms in optical lattices.[19,20] Intriguing quantum phases, including supersolid (with coexisting diagonal and off-diagonal long-range orders), valence-bond solid, and striped phases, have been found.[9–12,18] It has been checked that there is no stable supersolid (SS) phase in the simplest hard-core Bose-Hubbard model with only the nearest-neighbor interactions in a square lattice due to the solid-superfluid phase separation (PS). To stabilize a supersolid on the square lattice, the next-nearest-neighbor interaction is included, and in this case a striped supersolid appears.[2] Besides the next-nearest-neighbor interactions, the lattice frustration may also stabilize a supersolid against the PS. This has been shown in the hard-core Bose-Hubbard model on the isotropic triangular lattice around half filling,[9–12] however, the supersolid phase is not favored in more complicated frustrated lattices such as the Kagome lattice.[18] Therefore, it will be interesting to investigate the effects of lattice frustration on the possible supersolid phases.

Another importance of studying the Bose-Hubbard model comes from the fact that the model can be mapped to the spin-1/2 XXZ model in an external magnetic field via Matsubara-Matsuda transformation.[21] The possibility to realize a supersolid phase in spin models is also of great interest as these quantum spin systems may be realized in real materials,[5,22] and indeed a supersolid phase in the dimer-based frustrated quantum magnets has been reported very recently.[23–27]

In this paper, we investigate the effects of lattice frustration on supersolidity by studying the hard-core boson model on an anisotropic triangular lattice. The geometric frustration or the anisotropic strength is described by the ratio t'/t between the intrachain nearest-neighbor hopping t' and the interchain hopping t [see Fig. 1(a)]. We find that for small values of anisotropy ratio t'/t, a solid state emerges at $\rho=1/2$ and a supersolid is unstable toward phase separation due to the domain-wall proliferation mechanism. These behaviors are similar to those of a square lattice without frustration. For large values of anisotropy ratio t'/t, solid states emerge at $\rho=1/3,2/3$ and a supersolid phase appears in the region $\rho<2/3$. In particular, for intermediate values of anisotropy ratio t'/t, three kinds of solid states, with respect to the filling factors $\rho=1/3$, 1/2, and $\rho=2/3$ coexist. In this case, no stable SS is observed in our calculations. In addition, we observe solid-superfluid-supersolid transitions at half filling as the geometric frustration t'/t is increased.

II. MODEL AND METHOD

We consider the extended hard-core Bose-Hubbard model with nearest-neighbor interactions on an anisotropic triangular lattice,

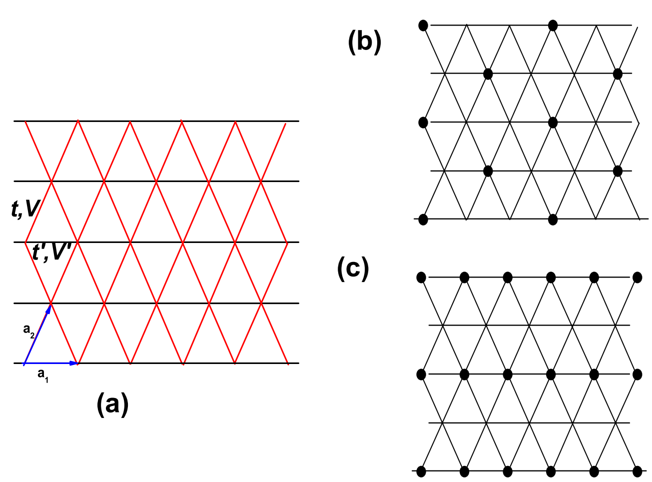

FIG. 1. (Color online) (a) Schematic structure of 2D anisotropic triangular lattice. The hopping integral and the repulsive interaction are t and V along a_2, t' and V' along a_1. a_1, a_2 denote the primitive vectors. (b) The solid state at $\rho=1/3$ for the isotropic triangular lattice $t'/t=1$. (c) The solid state at $\rho=1/2$ for $t'/t=0$.

$$H = -t\sum_{\langle ij\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + V\sum_{\langle ij\rangle} n_i n_j - \mu \sum_i n_i$$
$$- t'\sum_{(ij)}(a_i^\dagger a_j + a_j^\dagger a_i) + V'\sum_{(ij)} n_i n_j, \quad (1)$$

where $a_i^\dagger$ (a_i) is the creation (annihilation) operator of the bosonic atom at site i, $n_i = a_i^\dagger a_i$ is the number operator, and μ is the chemical potential. (ij) ($<ij>$) runs over the nearest-neighbor sites along the chain (between different chains), and the corresponding nearest-neighbor hopping integrals (repulsive interactions) are denoted by t' (V') and t (V) [see Fig. 1(a)].

The model has two limiting cases. At $t'/t=1$, the model reduces to an isotropic-triangular-lattice model with highly geometric frustration. In the classical limit $(t,t'=0)$, two solid states exist at fillings $\rho=1/3$ and $\rho=2/3$, where one or two of three sites is filled in a $\sqrt{3}\times\sqrt{3}$ ordering with wave vector $Q_1=(4\pi/3,0)$. When a small hopping parameter t is turned on, the system exhibits a supersolid phase at fillings $1/3<\rho<2/3$.[9–12] The emergence of a supersolid on the isotropic triangular lattice can be viewed as arising from an order-by-disorder mechanism, in which an extensive degeneracy of the classical ground states is lifted by quantum fluctuations (finite hopping t).[28] When t dominates, a uniform superfluid phase emerges.

At $t'/t=0$, the model is topologically equivalent to a square lattice without frustration. At half filling, the ground state is a checkerboard solid, where one of two sites is filled with wave vector $Q_2=(2\pi,0)$ [see Fig. 1(c); this is a little different from a square lattice, where the $\rho=1/2$ solid realizes a $\sqrt{2}\times\sqrt{2}$ ordering with wave vector (π,π)]. In the hard-core case, a supersolid phase is unstable toward phase separation.[2]

These two limiting cases (square and isotropic triangular lattice) have been studied a lot before. In this paper we focus our study on the anisotropic case. We set $\alpha=t'/t=V'/V$, where $0\le\alpha\le 1$ represents the anisotropic strength for an anisotropic triangular lattice. In the classical limit $(t,t'=0)$, a meaningful chemical potential is $\mu>0$, or otherwise no bosons are present. Increasing the chemical potential, several kinds of solid phases at fillings $\rho=1/3$, 1/2, 2/3 may emerge, depending on the value of the anisotropic strength t'/t. At even larger μ ($\mu>4V+2V'$), the lattice is completely filled with density $\rho=1$. In the hard-core limit, due to the particle-hole symmetry, the results are symmetric with respect to $\mu/V=2+\alpha$. Hereafter we set $V=1$ and use V as the energy unit.

The method we employ is the stochastic series expansion (SSE) quantum Monte Carlo (QMC) method with directed loop update.[29–33] We now portray our QMC simulations. In order to characterize different phases, we evaluate the static structure factor $S(Q)$ and the superfluid density ρ_s,

$$S(Q) = \frac{1}{N}\sum_{ij} e^{iQ\cdot(r_i-r_j)}\langle n_i n_j\rangle,$$

$$\rho_s^a = \frac{\langle W_a^2\rangle}{4\beta}, \quad (2)$$

where W is the winding number fluctuation of the bosonic world lines,[34] β is the inverse of fictitious temperature, a labels the a_1 or a_2 direction (see Fig. 1), and $N=L\times L$ is the lattice size. In order to distinguish different solid phases, we calculate the static structure factors at wave vectors $Q_1=(4\pi/3,0)$ and $Q_2=(2\pi,0)$, respectively. A SF phase is characterized by $S(Q)=0$ and $\rho_s\neq 0$; a SS phase is depicted by nonvanishing both $S(Q)$ and ρ_s; a $\rho=1/2$ checkerboard solid phase by $S(Q_1)=0$, $\rho_s=0$ and $S(Q_2)\neq 0$; a $\rho=1/3$ (and $\rho=2/3$) solid by $S(Q_1)\neq 0$, $\rho_s=0$ and $S(Q_2)=0$.

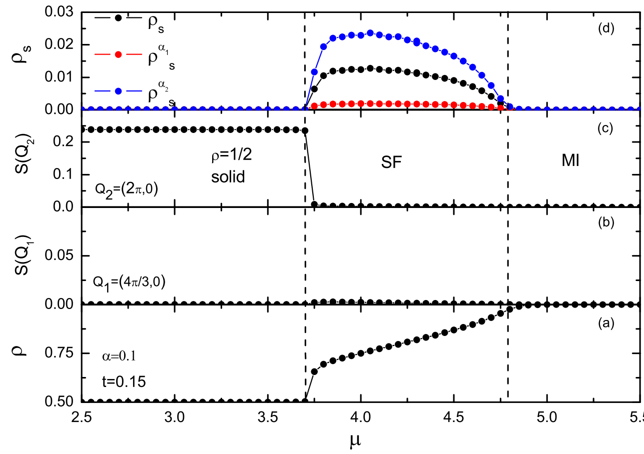

FIG. 2. (Color online) (a) The boson density ρ, (b) the structure factors $S(Q_1)$, (c) $S(Q_2)$, (d) the superfluid ρ_s as functions of the chemical potential μ for $\alpha=t'/t=V'/V=0.1$, $t/V=0.15$ with $n=12$ and $\beta=24$, respectively.

III. RESULTS AND DISCUSSION

We begin with the case for a small α. Figure 2(a) shows the boson density ρ as a function of the chemical potential μ for $\alpha=0.1$ and $t/V=0.15$. The $\rho=1/2$ solid plateau is clearly observed while the $\rho=1/3$ and $\rho=2/3$ solid plateaux do not exist. A jump in ρ, which indicates a first-order phase transition, appears on approaching $\rho=1/2$ from above. Figures 2(b)–2(d) show the static structure factor $S(Q)$ with $Q_1=(4\pi/3,0)$, $Q_2=(2\pi,0)$, and the superfluid density ρ_s as functions of μ for $\alpha=0.1$, respectively. A pronounced anisotropy of ρ_s is observed. For $\mu/V<3.7$, the ground state of the system is the $\rho=1/2$ solid with $\rho_s=0$ while $S(Q_2)\neq 0$; for $3.7<\mu/V<4.8$, the ground state is a superfluid phase with $\rho_s\neq 0$ while $S(Q)=0$; at the critical point $\mu_C/V\sim 3.7$, both ρ_s and $S(Q_2)$ exhibit a sudden jump, confirming the first-order phase transition; for $\mu/V>4.8$, both ρ_s and $S(Q)$ are zero with $\rho=1$, and the ground state is a Mott insulator. There is no region for both $S(Q)$ and ρ_s nonzero, i.e., no stable supersolid state. For small values of α, the results are similar to those obtained for a square lattice.[35]

In contrast, for a large α, the behaviors are quite different. Figure 3(a) shows the boson density as a function of μ for $\alpha=0.9$ and $t/V=0.15$. We can see that except the Mott insulator, there are $\rho=1/3$, 2/3 solid states while the $\rho=1/2$ solid state does not exist. In this case, there is a jump in ρ above $\rho=2/3$, indicating a first-order phase transition; while it is continuous below $\rho=2/3$, indicating a continuous phase transition. Figures 3(b)–3(d) show $S(Q)$ and ρ_s as functions

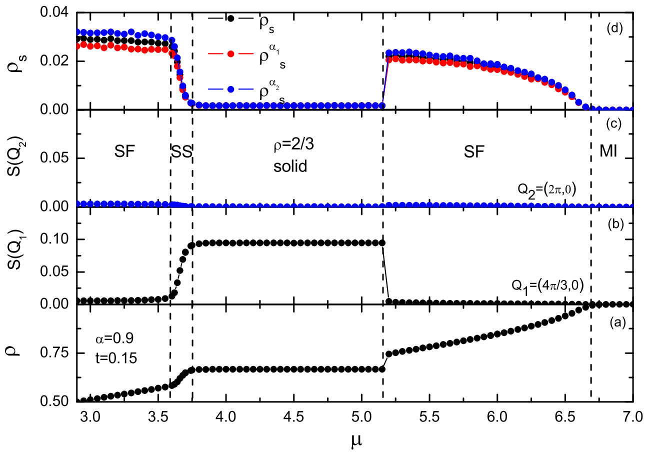

FIG. 3. (Color online) (a) The boson density ρ, (b) the structure factors $S(Q_1)$, (c) $S(Q_2)$, (d) the superfluid ρ_s as functions of the chemical potential μ for $\alpha=0.9$, $t/V=0.15$ with $n=12$ and $\beta=24$, respectively.

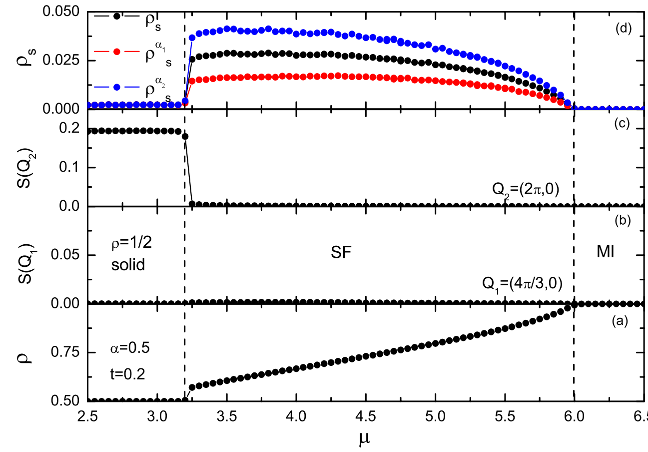

FIG. 5. (Color online) (a) The boson density ρ, (b) the structure factors $S(Q_1)$, (c) $S(Q_2)$, (d) the superfluid ρ_s as functions of the chemical potential μ for $\alpha=0.5$, $t/V=0.2$ with $n=18$ and $\beta=36$, respectively.

of μ, respectively. The anisotropy of ρ_s is quite weak as $t' \sim t$. In the density region around $\rho=1/2$, the structure factor $S(Q)=0$ while the superfluid density $\rho_s \neq 0$. The ground state is a SF. In the density region near $\rho=2/3$ ($\rho<2/3$), both $S(Q_1)$ and ρ_s are nonzero, i.e., a supersolid phase emerges. This behavior is a little different from that in the isotropic triangular lattice, where a supersolid phase exists everywhere between the $\rho=1/3$ and the $\rho=2/3$ solid. The finite-size scaling of ρ_s and $S(Q)$ for $\alpha=0.9$, $t/V=0.15$ is demonstrated in Fig. 7(a). For $\mu=3.65$ (near $\rho=2/3$), both ρ_s and $S(Q_1)$ are finite in the thermodynamic limit, confirming the survival of the supersolid phase. In the superfluid phase (around half filling), such as $\mu=3.25$, $S(Q)$ extrapolates to zero while ρ_s is finite.

Now we begin to study the intermediate anisotropy. Figure 4 shows the results for $\alpha=0.5$ and $t/V=0.175$. The boson density ρ as a function of μ is shown in Fig. 4(a). We can see

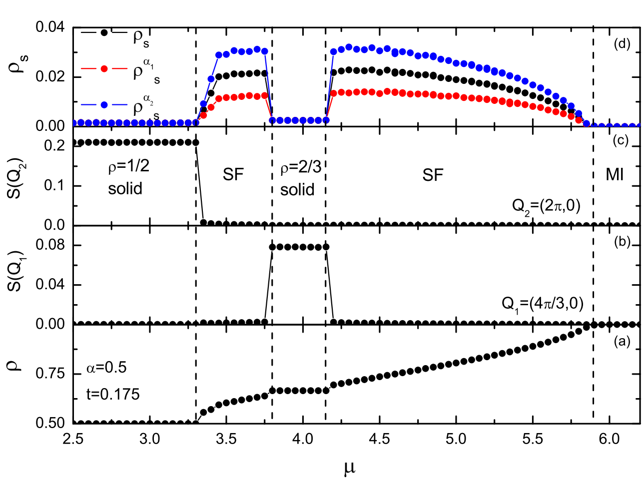

FIG. 4. (Color online) (a) The boson density ρ, (b) the structure factors $S(Q_1)$, (c) $S(Q_2)$, (d) the superfluid ρ_s as functions of the chemical potential μ for $\alpha=0.5$, $t/V=0.175$ with $n=18$ and $\beta=36$, respectively.

that for $\alpha=0.5$, both the $\rho=1/2$ solid plateau and the $\rho=1/3,2/3$ solid plateaux exist, and the $\rho=1/2$ solid plateau is much larger than that of $\rho=1/3,2/3$. Figures 4(b)–4(d) show $S(Q)$ and ρ_s as functions of μ, respectively. Jumps are observed at each critical point, i.e., from the $\rho=1/2$ solid to the $\rho>1/2$ SF and from the $\rho=2/3$ solid to the $\rho>2/3(\rho<2/3)$ SF. For $\alpha=0.5$, we find no region for both superfluid and structure factors nonzero, i.e., there is no stable supersolid phase.

In Fig. 5, with slightly larger $t/V=0.2$, the $\rho=1/2$ solid is still observed while the $\rho=2/3$ solid disappears. Both the structure factors and the superfluid density are discontinuous at the transition point $\mu/V\sim3.2$. This indicates a first-order phase transition from the $\rho=1/2$ solid to the SF, and also there is no stable supersolid phase.

To further investigate the effects of frustration on the formation of a supersolid, we measure the anisotropy dependence at half filling. As we have discussed above, model (1) is symmetric with respect to $\mu=2+\alpha$ due to the particle-hole symmetry. Below we focus our study at half filling, and choose $\mu=2+\alpha$. Figure 6 shows the superfluid ρ_s and the structure factors $S(Q)$ as functions of the anisotropic strength α at half filling. With increasing α, we observe phase transitions from the $\rho=1/2$ solid phase to the $\rho=1/2$ SF phase and then to the $\rho=1/2$ SS phase. For $\alpha<0.83$, $\rho_s=0$ and $S(Q_1)=0$ while the structure factor $S(Q)$ at ordering wave vector $Q_2=(2\pi,0)$ is nonzero. The ground state is a $\rho=1/2$ checkerboard solid. For $0.83<\alpha<0.9$, $\rho_s\neq0$ while $S(Q_1)=0$ and $S(Q_2)=0$. The ground state is a superfluid phase. For $\alpha>0.9$, $S(Q_2)$ is zero, while both the superfluid density ρ_s and the structure factor $S(Q)$ at ordering wave vector $Q_1=(4\pi/3,0)$ are nonzero. The ground state is a stable supersolid phase at half filling. The finite-size scaling of ρ_s and $S(Q)$ at half filling is shown in Fig. 7(b). For $\alpha=0.88$, both $S(Q_1)$ and $S(Q_2)$ extrapolate to zero in the thermodynamic limit, revealing the absence of a supersolid; while for $\alpha=0.98$ (quite close to the isotropic limit), both $S(Q_1)$ and ρ_s extrapolate to finite values, confirming the existence of a supersolid. This indicates that for a two-dimensional aniso-

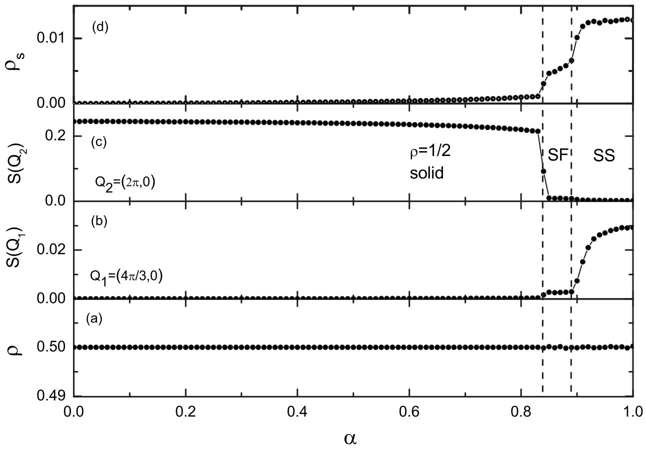

FIG. 6. (a) The boson density ρ, (b) the structure factors $S(Q_1)$, (c) $S(Q_2)$, (d) the superfluid ρ_s as functions of the anisotropic strength $\alpha=t'/t=V'/V$ at half filling $(\mu=2+\alpha)$ for $t/V=0.1$ with $n=12$ and $\beta=24$. There are phase transitions from the $\rho=1/2$ solid phase to the superfluid phase at around $\alpha=0.83$ and then to the supersolid phase at around $\alpha=0.9$.

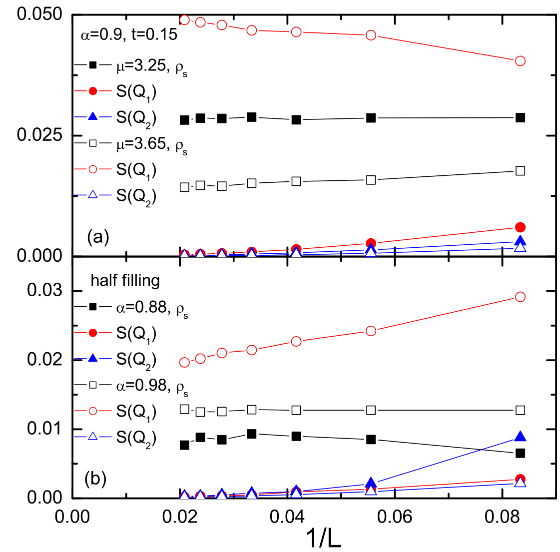

FIG. 7. (Color online) Finite-size scaling of the superfluid density ρ_s and the static structure factor $S(Q)$ (a) for $\mu=3.25,3.65$ with $\alpha=0.9$, $t/V=0.15$ (see Fig. 3); (b) for $\alpha=0.88,0.98$ at half filling (see Fig. 6). The inverse temperature $\beta=36$.

tropic triangular lattice with nearest-neighbor interactions, a supersolid phase survives only around the isotropic limit.

IV. CONCLUSION

We have studied the hard-core Bose-Hubbard model with nearest-neighbor interactions on an anisotropic triangular lattice by using the quantum Monte Carlo simulations. The effects of the geometric frustration or the anisotropic strength, characterized by the ratio t'/t between the intrachain nearest-neighbor hopping t' and the interchain hopping t, are presented. We find that for small values of anisotropy ratio t'/t, a solid state emerges at $\rho=1/2$ and a supersolid is unstable toward phase separation. These behaviors are similar to those of a square lattice without frustration. For large values of anisotropy ratio t'/t, solid states emerge at $\rho=1/3$, 2/3 and a supersolid phase is stable in the region $\rho<2/3$. In addition, for intermediate values of anisotropy ratio t'/t, three kinds of solid states at fillings $\rho=1/3,1/2,2/3$ coexist and no stable supersolid phase is observed.

At half filling, we find solid-superfluid-supersolid transitions as the geometric frustration t'/t is increased. In particular, we find that the supersolid phase survives only in a narrow region near the isotropic limit $(t'/t=1)$. This means that the supersolid phase that appears in the isotropic limit is rather unstable under the presence of a small anisotropy. These results provide the requirement for finding the supersolid phases in real systems, i.e., the systems have to be quite close to the isotropic triangular limit with highly geometric frustration.

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