

Supersolid order of frustrated hard-core bosons in a triangular lattice system

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(Received 26 December 2008; published 30 January 2009)

We numerically demonstrate that a supersolid phase exists in a frustrated hard-core boson system on a triangular lattice over a wide range of interaction strength. In the infinite repulsion (Ising) limit, we establish a mapping to the same problem with unfrustrated hopping, which connects the supersolid to the known results in that case. The weak superfluidity can be destroyed or strongly enhanced by a next-nearest-neighbor hopping term, which provides valuable information for experimental realization of a supersolid phase on optical lattice. A phase diagram for the frustrated anisotropic Heisenberg model on triangular lattice is also established.

DOI: 10.1103/PhysRevB.79.020409

PACS number(s): 75.10.Jm, 03.75.Lm, 05.30.Jp

I. INTRODUCTION

A supersolid phase is a state of matter exhibiting both diagonal and off-diagonal long-range order (ODLRO).¹ Recent possible observation of a supersolid phase² in ⁴He under pressure has attracted a lot of interest. While the microscopic conditions under which clean ⁴He could be in a supersolid phase are still unclear, supersolidity is established for hard-core bosons on a triangular lattice, which is the focus of many recent studies.³⁻⁷ The supersolid phase is an example of ordering by disorder demonstrated for hard-core boson system with unfrustrated nearest-neighbor (NN) hopping and strong repulsion⁴⁻⁶ based on extensive quantum Monte Carlo simulations and theoretical analysis. These theoretical works are motivated in part by experimental realizations of lattice bosons in ultracold atom traps.⁸ Intriguingly, the superfluid density in the supersolid phase is found to be very small, possibly indicating that the system is near a phase boundary⁹ to an insulating phase. It is thus highly desirable to examine the stability of the supersolid phase in more extended models to determine the relevant perturbation and possibly to suggest a route of getting into a deep supersolid phase for experiment.

The nature of the state for the hard-core bosons with *frustrated* NN hopping on triangular lattice is another open issue, where the model can be mapped to the spin-1/2 XXZ antiferromagnetic (AF) Heisenberg model which suffers from the sign problem. Historically this model was the first candidate proposed to realize a spin liquid ground state,¹⁰ although it turns out to still exhibit a three-sublattice AF long-range-order (LRO) in general, which may persist to large J_z limit.¹¹ However, extensive numerical studies have been limited to near the SU(2) point¹² and the precise nature of the ordering at larger J_z (or the strong NN repulsion limit for the corresponding boson model) has not been well understood.

In this Rapid Communication, we present a systematic density-matrix renormalization-group (DMRG) and exact diagonalization (ED) numerical studies of the half-filled ground state of the *frustrated* model over a wide range of the NN repulsion. We show that a robust supersolid phase does exist in this model and it can be related to the well-known

supersolid phase of an unfrustrated NN hopping model in infinite repulsion (Ising) limit, where a precise mapping between the two models by a sign transformation can be established. Furthermore, we reveal that the supersolid phase is close to a transition to an insulating phase, and correspondingly the superfluidity can be strongly enhanced (or easily switched off) by tuning a next-nearest-neighbor (NNN) hopping term. Our results have also provided a theoretical understanding of the nature of the ground state of the frustrated Heisenberg model on triangular lattice at the large J_z limit.

II. SUPERSOLID PHASE FROM ISOTROPIC SU(2) POINT TO LARGE J_z LIMIT

We consider a simple model of hard-core bosons at half-filling on the triangular lattice interacting via a repulsive term,

$$H = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + \sum_{\langle ij \rangle} V \left(n_i - \frac{1}{2} \right) \left(n_j - \frac{1}{2} \right), \quad (1)$$

where b_i^\dagger is a boson creation operator and n_i is a boson number operator. $\langle ij \rangle$ denotes NN sites and we shall mainly consider the frustrated boson hopping at $t < 0$. This boson Hamiltonian is equivalent to—by a standard mapping from hard-core bosons to $S=1/2$ spins—an XXZ Heisenberg model on the triangular lattice,

$$\mathcal{H} = \sum_{\langle ij \rangle} \left[\frac{J_\perp}{2} (S_i^x S_j^x + \text{H.c.}) + J_z S_i^z S_j^z \right], \quad (2)$$

with $J_z = V$ and $J_\perp = -2t$. In the spin language, a charge-density wave (solid) order implies infinite-range correlations of the z component of spins at a nonzero wave vector, while the superfluid order is equivalent to the in-plane ordering of the spins also at a nonzero wave vector for the frustrated system. In the following analysis, we will work interchangeably in terms of bosons and spin variables.

We first present the numerical results based on DMRG method¹³ for a triangular lattice with the total number of sites $N = N_1 \times N_2$. We keep up to $m = 4096$ states in each DMRG block for most systems and the truncation error is of the

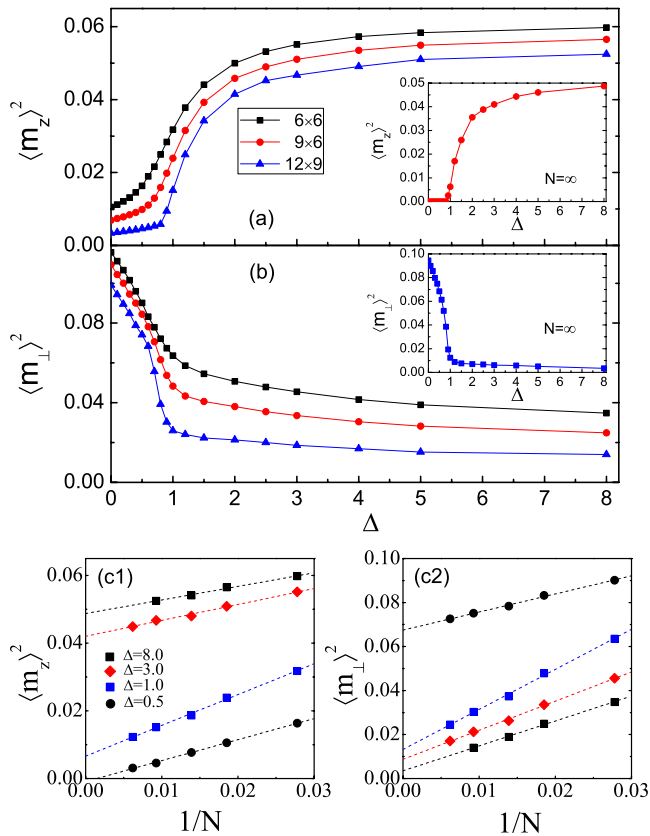


FIG. 1. (Color online) The order-parameter squared, $\langle m_z \rangle^2$ and $\langle m_{\perp} \rangle^2$, as functions of the anisotropy $\Delta = J_z/J_{\perp}$ are shown in (a) and (b), respectively, with $N = 6 \times 6$, 9×6 , and 12×9 . The insets are the corresponding extrapolations in the thermodynamic limit. Examples of finite-size scaling of the order parameters are also shown in (c1) and (c2) with system size up to $N = 9 \times 18$.

order or less than 10^{-5} . We make use of the periodic boundary condition to reduce the finite-size effect for a more reliable extrapolation to the thermodynamic limit. To analyze the magnetic properties of the system, we calculate the structure factors $S_z(\mathbf{q})$ and $S_{\perp}(\mathbf{q})$ defined by $S_z(\mathbf{q}) = \frac{1}{N} \sum_{i,j} e^{-i\mathbf{q}(\mathbf{r}_i - \mathbf{r}_j)} \langle S_i^z S_j^z \rangle$ and $S_{\perp}(\mathbf{q}) = \frac{1}{N} \sum_{i,j} e^{-i\mathbf{q}(\mathbf{r}_i - \mathbf{r}_j)} \langle S_i^+ S_j^- \rangle$.

The obtained $S_z(\mathbf{q})$ and $S_{\perp}(\mathbf{q})$ show Bragg peaks at the corners of the hexagonal Brillouin zone [e.g., at $q_0 = (\pm 4\pi/3, 0)$]. In particular, at small $\Delta \equiv J_z/J_{\perp} < 1$, the peak of $S_z(\mathbf{q}_0)$ is very weak, while that of $S_{\perp}(\mathbf{q}_0)$ is very sharp, representing the dominant AF correlation in the XY plane. With the increase of Δ , $S_z(\mathbf{q}_0)$ grows continuously and its value becomes bigger than the in-plane ones passing the point $\Delta = 1$. One can obtain the magnetic order parameters based on the finite-size scaling of the peak values of $S_z(\mathbf{q}_0)$ and $S_{\perp}(\mathbf{q}_0)$. Specifically, the average magnetization $\langle m_z \rangle$ and $\langle m_{\perp} \rangle$ can be determined by $\langle m_z \rangle^2 = S_z(\mathbf{q}_0)/N$ and $\langle m_{\perp} \rangle^2 = S_{\perp}(\mathbf{q}_0)/N$, which are shown vs Δ at $N = 36, 54$, and 108 in the main panel of Figs. 1(a) and 1(b).

Nonzero $\langle m_z \rangle^2$ and $\langle m_{\perp} \rangle^2$ in the thermodynamic limit will correspond to the diagonal LRO and ODLRO, respectively. Examples of the finite-size scaling are shown in Figs. 1(c1) and (c2) by plotting $\langle m_z \rangle^2$ and $\langle m_{\perp} \rangle^2$ as functions of $1/N$. Thus obtained order parameters extrapolated to the thermodynamic limit are presented in the insets of Figs. 1(a) and

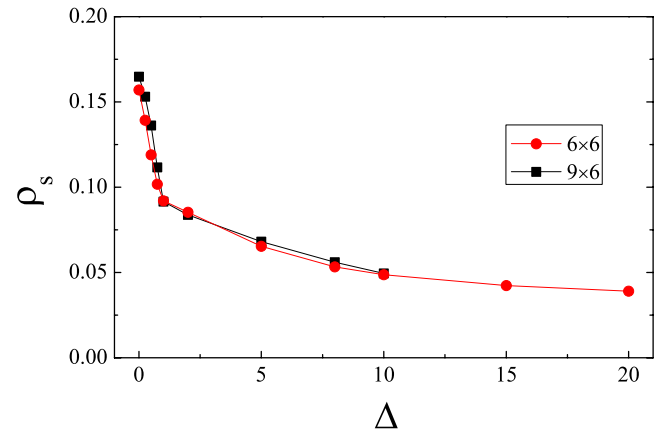


FIG. 2. (Color online) Superfluid stiffness ρ_s (in units of J_{\perp}) as a function of the anisotropy $\Delta = J_z/J_{\perp}$ obtained from ED ($N = 36$) or DMRG ($N = 54$) calculations.

1(b). At small Δ , the system is in the pure superfluid phase with magnetic order solely lying in the XY plane with $\langle m_{\perp} \rangle^2 \neq 0$ and $\langle m_z \rangle = 0$ (cf. the inset of Fig. 1). By contrast, at $\Delta > 1$ the three-sublattice antiferromagnetic long-range order develops in both z direction and XY plane characterized by nonzero values of $\langle m_z \rangle^2$ and $\langle m_{\perp} \rangle^2$. Here $\langle m_z \rangle$ monotonically increases with Δ from the isotropic point ($\Delta = 1$) consistent with the spin-wave picture of coplanar ordering in the XZ plane. For the corresponding boson system, our results suggest a supersolid phase with coexisting diagonal LRO and ODLRO at $\Delta \geq \Delta_c$. The phase boundary Δ_c between the superfluid phase and supersolid phase is very close to the isotropic point $\Delta_c = (J_z/J_{\perp})_c = (V/2|t|)_c \sim 1.00$.

We note that at large J_z case, e.g., $\Delta = 8$, $\langle m_z \rangle^2 = 0.049$ ($\langle m_z \rangle = 0.24$) which is much larger than the corresponding value at the isotropic point, while the XY-plane magnetization reduces to $\langle m_{\perp} \rangle^2 = 0.0036$ ($\langle m_{\perp} \rangle = 0.06$) in the thermodynamic limit. Though this superfluid ordering is small, its value actually is comparable with that of the unfrustrated hard-boson supersolid⁴⁻⁶ at the same large J_z limit as we have checked numerically. In the following, we can further establish the presence of the superfluidity through the calculation of the superfluid density ρ_s by adding a nonzero twist phase at the system boundary with $\rho_s = \frac{\partial^2 E}{\partial \theta_x^2} \propto [E(\theta_x = \pi) - E(\theta_x = 0)]$. We obtain ρ_s by adding a twist phase $\theta_x = \pi$ in both ED and DMRG calculations,¹⁴ which are shown in Fig. 2 as a function of Δ for $N = 36$ and $N = 54$. From the figure, we can see that the finite-size effect for ρ_s is very weak and ρ_s should remain finite in the thermodynamic limit consistent with the finite $\langle m_{\perp} \rangle^2$ in Fig. 1. At $J_z > 10$, the DMRG becomes difficult to converge as the energy from J_z term becomes dominant; the ED results further suggest that the obtained ρ_s should be nonzero over the whole range of J_z with a value matching with the ones for the unfrustrated bosons in the large J_z limit.⁶

III. SUPERSOLID ORDER IN THE ISING LIMIT

Now we turn to the interesting limit of $\Delta \rightarrow \infty$, where the direct in-plane magnetic ordering in the numerical results is

very weak and the spin-wave theory suggests that it vanishes as square root of J_{\perp}/J_z . Clearly, here a rigorous examination is desired. At $J_z \rightarrow \infty$, the XXZ model in Eq. (2) reduces to the classical Ising AF on a triangular lattice. This classical model is well known to have a macroscopic degeneracy of ground states, which correspond to all spin configurations with exactly one frustrated bond per triangle.¹⁵ In this limit, the XXZ model reduces to

$$H_{\infty} = J_{\perp}/2 \sum_{\langle ij \rangle} \hat{P}_C (S_i^+ S_j^- + \text{H.c.}) \hat{P}_C, \quad (3)$$

where \hat{P}_C is a projection operator onto the classical Ising ground-state manifold.

The unfrustrated model with $J_{\perp} < 0$ has been studied previously and shown to exhibit supersolid order.⁴⁻⁶ We now show how supersolidity in the frustrated case $J_{\perp} > 0$ can be deduced from those known results. We first consider thermodynamic and other properties that can be deduced from the partition function and *diagonal* expectation values of the form,

$$Z(\mathcal{O}; J_{\perp}) = \text{Tr} \{ \hat{P}_C \mathcal{O} [(S_i^z)] e^{-\beta H_{\infty}} \}, \quad (4)$$

where \mathcal{O} is any function of the z components of the spins (including the identity operator where Z reduces to the partition function). From such quantities, we can calculate the free energy and the diagonal (solid) correlations. We show that Z is an *even* function of J_{\perp} , and so these properties are identical for the frustrated and unfrustrated cases. To see this, consider the high-temperature expansion of Z in powers of βJ_{\perp} . The terms in the expansion consist of successive actions of bond operators of the form $\hat{P}_C S_i^+ S_j^- \hat{P}_C$ on nearest-neighbor links, with a factor of βJ_{\perp} accompanying each bond operator. To achieve a nonzero expectation value in the trace, the boson number on each site must be unchanged after the action of all these operators. Graphically, we may represent each factor of $S_i^+ S_j^-$ on the lattice as an arrow pointing from site j to site i , and we require this ‘‘vector field’’ to have zero divergence, i.e., the arrows close into ‘‘exchange’’ loops. Now consider the contribution from any particular state in the trace. Due to the projection, each bond operator has a nonzero action only if i and j are ‘‘flippable,’’ i.e., the two other spins on each triangle containing i or j are antiparallel. Now let us circumscribe each exchange loop on our graphical representation by a neighboring loop as in Fig. 3. In order that all sites on the exchange loops are flippable, spins on the neighboring loops must alternate, which requires that all of the neighboring loops must have an *even* number of sites. This in turn requires that the total number of links on each exchange loop is even. Thus $Z[\mathcal{O}; J_{\perp}]$ is indeed an even function of J_{\perp} .

Now consider the off-diagonal correlation function,

$$\langle S_j^+ S_i^- \rangle = Z^{-1} \text{Tr} [\hat{P}_C S_j^+ S_i^- e^{-\beta H_{\infty}}]. \quad (5)$$

Once again, one may consider the high-temperature expansion of the numerator (the denominator Z has already been shown to be even). In this case, contributions must be divergenceless *except* at the sites i and j , which appear as source and sink, respectively. One can understand the behavior by

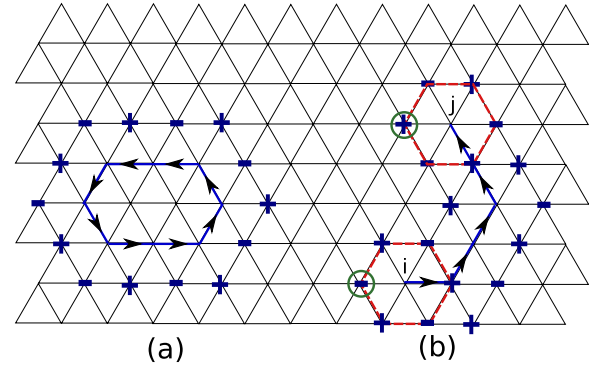


FIG. 3. (Color online) Illustration of the paths contributing to the high-temperature expansion and the associated sign rule. In (a), we show a representative loop appearing in the expansion of the partition function. The \pm signs show one of two alternating spin configurations allowed around the loop, which allows only even-length loops. In (b), we show a representative path in the expansion of the off-diagonal correlation function between sites i and j . For such a path with an odd number of steps, the auxiliary sites $i + \hat{a}, j + \hat{a}$ (shown in circles) must be antiparallel.

considering just the simplest terms, in which the arrows form a single path connecting i to j (see Fig. 3). Now form a tightly circumscribing loop about this path. As above, for any state in the trace to contribute, the spins S_k^z on the sites of this neighboring loop must alternate. Moreover, the six spins neighboring i and j must also alternate since $S_j^+ S_i^-$ acts directly on these states. Now consider the product $4S_{i+\hat{a}}^z S_{j+\hat{a}}^z$, where \hat{a} is any nearest-neighbor vector, acting on a state which contributes to the trace. Because of the alternating spins around the circumscribing loop, this factor gives the parity of the exchange path, i.e., it equals $+1$ for an even path and -1 for an odd path. One may show that this conclusion is unaffected by additional closed loops, which appear as higher-order terms in the high-temperature series. Since this is true for every term in the expansion, we find $\langle S_j^+ S_i^- \rangle |_{J_{\perp} > 0} = \langle 4S_{i+\hat{a}}^z S_{j+\hat{a}}^z S_j^+ S_i^- \rangle |_{-J_{\perp}}$.

The above observations lead us to the conclusion that the supersolid phase survives even for the frustrated hard-core boson system at strong repulsion ($V = J_z \rightarrow \infty$) limit as it maps to the unfrustrated model.⁴⁻⁶

IV. ENHANCEMENT OF THE SUPERFLUIDITY AND THE ORDERING OF THE SUPERSOLID PHASES

To understand the underlying reason why the superfluid stiffness is relatively weak,⁹ we add a NNN hopping $t' = -J'/2$ term. For simplicity we only present the results for $J_{\perp} = -2t > 0$ and large J_z (Ising) limit, although the obtained results also apply to both models with a finite range of J_z .

The superfluid stiffness is calculated using the ED method for the projected Hamiltonian. As illustrated in Fig. 4, ρ_s is relatively small at $J' = 0$ compared to its value in the region $J'/J_{\perp} < 0$ (negative sign represents an unfrustrated NNN hopping). In fact, ρ_s monotonically increases with a negative J' and when $J' = -J_{\perp}$, ρ_s becomes comparable to the value of a pure superfluid phase (i.e., the ferromagnetic XY model on

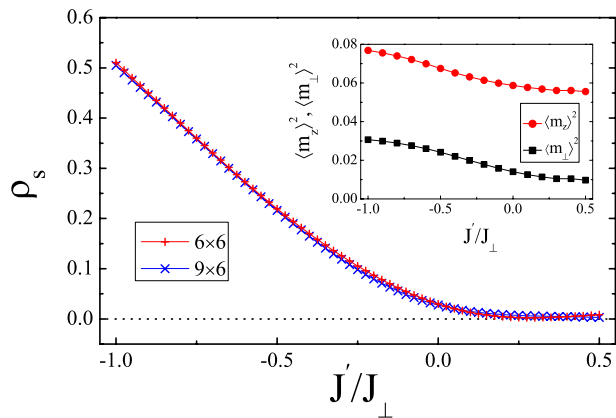


FIG. 4. (Color online) Superfluid stiffness ρ_s (in units of J_\perp) vs J'/J_\perp for systems with NNN hopping t' (superexchange J'). The finite-size order parameters $\langle m_z \rangle^2$ and $\langle m_\perp \rangle^2$ at $N=54$ are shown in the inset.

triangular lattice⁶). Clearly a boson system at $J'=0$ is indeed near the phase boundary of an insulating phase, which occurs at $(J'/J_\perp)_c \sim 0.2$ (which we further identify as a solid phase with diagonal LRO). The finite-size order parameters $\langle m_z \rangle^2$ and $\langle m_\perp \rangle^2$ for $N=54$ are also shown in the inset of Fig. 4, where the enhancement of the peaks of the structure factors $S_z(q_0)$ and $S_\perp(q_0)$ are clearly seen as we continuously turn on the negative J' . Thus the resulting phase is a supersolid phase with strong diagonal LRO and superfluidity.

These observations and the precise nature of the supersolid ordering can be rationalized by simple energetic arguments in the large J_z limit. For the NN hopping case ($J'=0$), the constraint that neighboring spins to the hopping path must alternate tends to enhance hopping that takes “60°” turns (forming hexagonal path), which keeps the bosons on two of the three sublattices. Moreover, the third sublattice on which hopping does not proceed must be substantially polarized. Thus the three-sublattice ordering $\langle S_z \rangle = (-m, -m, 2m + \delta)$ is favored energetically consistent with a ferrimagnetic-

ordered phase.^{7,16} When the NNN hopping term is dominant ($-J' \geq J_\perp$), bosons tend to hop on a single (say A) sublattice, while spins on the neighboring sites from sublattices B and C are individually preferred to be ferromagnetically aligned with B and C spins antiparallel to each other. This corresponds to $\langle S_z \rangle = (0, m, -m)$ or “antiferromagnetic” ordering, which we therefore expect in the large $-J'$ limit. This is indeed supported by numerics, which will be presented elsewhere.

In summary, we have established a robust supersolid phase for the frustrated hard-core bosons on a triangular lattice at half-filling based on extensive numerical calculations and analytical analysis. The observed supersolidity is an example of ordering by disorder elegantly realized for such a frustrated system. Furthermore, we have found that the supersolid phases for the hard-core boson models with only NN hoppings are quite close to a pure solid phase in both frustrated and unfrustrated cases. But a small unfrustrated NNN hopping term can push the boson systems into a deep supersolid phase with greatly enhanced superfluidity. Our theoretical study can thus provide a solid foundation for the experimental realization of supersolid phase on a triangular optical lattice.

ACKNOWLEDGMENT

The authors would like to thank R. G. Melko for insightful discussions. This work is supported by the NSFC under Grants No. 10688401 (H.C.J. and Z.Y.W.) and No. 10804103 (M.Q.W.), the National Program for Basic Research of MOST, China (Z.Y.W.), the DOE under Grant No. DE-FG02-06ER46305, the NSF under Grants No. DMR-0605696, No. DMR-0611562 (H.C.J. and D.N.S.), and No. DMR-0804564 (L.B.), and the Packard Foundation (L.B.). In finishing this work, we became aware of a parallel work¹⁶ which has reached similar conclusion based on different approaches. We are grateful to the author (A. V.) for sending us the preprint before submission.

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