Supersolid Hard-Core Bosons on the Triangular Lattice

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We determine the phase diagram of hard-core bosons on a triangular lattice with nearest-neighbor repulsion, paying special attention to the stability of the supersolid phase. Similar to the same model on a square lattice we find that for densities $\rho < 1/3$ or $\rho > 2/3$ a supersolid phase is unstable and the transition between a commensurate solid and the superfluid is of first order. At intermediate fillings $1/3 < \rho < 2/3$ we find an extended supersolid phase even at half filling $\rho = 1/2$. The emergence of the supersolid on the triangular lattice reflects a novel and interesting way for a quantum system to avoid classical frustration, similar to an order-by-disorder mechanism. It also offers an exciting possibility of realizing such phenomena in ultracold atoms on optical lattices.

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Next to the widely observed superfluid and Bose-condensed phases with broken $U(1)$ symmetry and "crystalline" density wave ordered phases with broken translational symmetry, the supersolid phase, breaking both the $U(1)$ symmetry and translational symmetry, has been a widely discussed phase that is hard to find both in experiments and in theoretical models. Experimentally, evidence for a possible supersolid phase in bulk ^{4}He has recently been presented [1], but the question of whether a true supersolid has been observed is far from being settled [2,3], leaving the old question of supersolid behavior in translation invariant systems [4,5] unsettled for now.

More precise statements for a supersolid phase can be made for bosons on regular *lattices*. It has been proposed that such bosonic lattice models can be realized by loading ultracold bosonic atoms into an optical lattice, where the required longer range interaction between the bosons could be induced by using the dipolar interaction in chromium condensates [6], or an interaction mediated by fermionic atoms in a mixture of bosonic and fermionic atoms [7]. With the recent realization of a Bose-Einstein condensate (BEC) in chromium atoms [8], these experiments have now become feasible, raising the interest in phase diagrams of lattice boson model, and particularly in the stability of supersolids on lattices.

The question if a supersolid phase is a stable thermodynamic phase for lattice boson models has been controversial for many years. Mean-field and renormalization group calculations [9–12] have predicted supersolid phases for many models, including the simplest model of hard-core bosons with nearest-neighbor repulsion on a square lattice with Hamiltonian

$$H = -t\sum_{\langle i,j\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + V\sum_{\langle i,j\rangle} n_i n_j - \mu\sum_i n_i, \qquad (1)$$

where $a_i^\dagger$ (a_i) creates (destroys) a particle on site i, t denotes the nearest-neighbor hopping, V a nearest-neighbor repulsion, and μ the chemical potential. Subsequent numerical investigations using exact diagonalization and quantum Monte Carlo (QMC) methods [13–17] have shown that for this model, the supersolid phase is unstable and phase separates into superfluid and solid domains at a first-order (quantum) phase transition. Recently, this occurrence of a first-order phase transition was explained by showing that a uniform supersolid phase in a hard-core boson model is unstable towards the introduction of domain walls, lowering the kinetic energy of the system by enhancing the mobility of the bosons on the domain wall [16]. In a related work it has been proposed that superfluid domain walls might be an explanation for the experimental observation of possible supersolidity in helium [3,18].

To stabilize a supersolid on the square lattice, the kinetic energy of the bosons in the supersolid has to be enhanced either by sufficiently reducing the on-site interaction to be less than $4V$ [16], by adding next-nearest-neighbor hopping terms [17], or by forming striped solid phases with longer-ranged repulsions [13,19].

In this Letter we consider the interplay of supersolidity and *frustration* by studying the hard-core boson model (1) on a *triangular* lattice. In the classical limit $t = 0$ two solid phases exist at fillings $\rho = 1/3$ (and $\rho = 2/3$), where one of three sites is filled (empty) in a $\sqrt{3} \times \sqrt{3}$ ordering with wave vector $\mathbf{Q} = (4\pi/3, 0)$ [20], shown in the insets of Fig. 1. At half filling ($\rho = 1/2$), where the square lattice shows a solid ordering with wave vector (π, π), the solid order is frustrated on the triangular lattice, and the classical model has a hugely degenerate ground state with an extensive zero-temperature entropy [21].

The question arises whether this degeneracy of the classical system at half filling is lifted when quantum dynamics is added at a finite hopping parameter t, and which phase gets stabilized. Mean-field studies have predicted a supersolid phase [22]. Given the questionable reliability of mean-field calculations in the case of the square lattice model a numerical check is needed.

We have thus performed a series of high-accuracy numerical QMC calculations on large lattices using stochastic series expansions [23] with global directed-loop updates

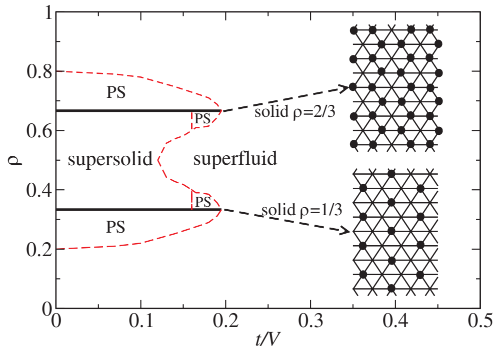

FIG. 1 (color online). Zero-temperature phase diagram of hard-core bosons on the triangular lattice in the canonical ensemble obtained from quantum Monte Carlo simulations. The regions of phase separation are denoted by PS. The insets exhibit the density distribution inside the solid phases for $\rho = 1/3$ (lower panel) and $\rho = 2/3$ (upper panel).

[24] for the hard-core boson model on the triangular lattice and show the phase diagram in Figs. 1 and 2 for the canonical and grand-canonical ensemble, respectively. The main results are that for fillings $\rho < 1/3$ and $\rho > 2/3$ a supersolid is unstable towards phase separation by exactly the same domain-wall proliferation mechanism through which the square lattice supersolid is unstable at all fillings $\rho \neq 1/2$. In contrast, for intermediate densities $1/3 < \rho < 2/3$ we find that the degeneracy of the frustrated classical model is indeed lifted and a stable supersolid phase emerges. The phase diagram in Fig. 2 is similar to the mean-field phase diagram [22], albeit with a substantially reduced supersolid region. The supersolid is stable even at half filling, contradicting the Green's function Monte Carlo results of Ref. [25], which are however intrinsically affected by a population size bias.

We will now discuss the phase diagrams in more detail, starting with simple limits. Considering the single boson (hole) problem, one can show that the lattice is empty for $\mu < \mu_0 = -6t$ and completely filled for $\mu > \mu_1 = 6(t + V)$. For large values of t/V, the bosons are superfluid, with a finite value of the superfluid density ρ_S, which we measure through the winding number fluctuations W of the world lines [26] as $\rho_S = \langle W^2 \rangle/(4\beta t)$. Two solid phases emerge upon lowering t/V with rational fillings $1/3$ and $2/3$, respectively. Both are characterized by a finite value of the density structure factor per site, $S(\mathbf{q})/N = \langle \rho_{\mathbf{q}} \rho_{\mathbf{q}}^\dagger \rangle$, where $\rho_{\mathbf{q}} = (1/N)\Sigma_i n_i \exp(i\mathbf{q} \cdot \mathbf{r}_i)$ at wave vectors $\pm\mathbf{Q} = \pm(4\pi/3, 0)$, corresponding to the $\sqrt{3} \times \sqrt{3}$ ordering wave vector. The maximum extent of the solid phases is reduced by quantum fluctuations from the mean-field value of $(t/V)_c = 0.5$ down to $(t/V)_c = 0.195 \pm 0.025$.

Since the phase diagram is symmetric when interchanging particles with holes ($\rho \to 1 - \rho$) we restrict our discussion from now on to $\rho \geq 1/2$ and plot the density ρ as a function of chemical potential μ for cuts at constant t/V in Fig. 3. For $t/V = 0.1$ we clearly observe a plateaux corresponding to the $\rho = 2/3$ phase with broken translational symmetry. The approach to this plateaux from $\rho < 2/3$ is continuous, indicating a second-order phase transition, while for $\rho > 2/3$ we see a jump caused by a first-order phase transition. Measuring the density structure factor $S(\mathbf{q})$ and the superfluid density in Fig. 4 we identify this as a first-order phase transition between the solid and superfluid phases.

The situation here is the same as in the square lattice model, where doping the solid leads to phase separation at a first-order phase transition [16]: the uniform supersolid is unstable towards domain-wall formation as illustrated in Fig. 5. Adding $L/3$ bosons onto the solid at density $\rho = 2/3$ [Fig. 5(a)] corresponds to an infinitesimal density in the thermodynamic limit. These bosons can gain a kinetic energy of $-6t^2/V$ per boson by second-order hopping processes. Placing these additional bosons along a line, as shown in Fig. 5(b), costs no additional potential energy, and we can even shift half of the lattice by one lattice spacing, introducing a domain wall as shown in Fig. 5(c), again at no potential energy cost. But now, the additional bosons gain kinetic energy of $-t$ per boson by hopping freely across the domain wall, which lowers the energy of the domain-wall state compared to the bulk supersolid, and hence the supersolid phase is unstable.

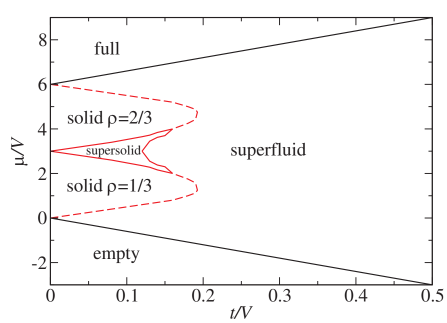

FIG. 2 (color online). Zero-temperature phase diagram of hard-core bosons on the triangular lattice in the grand-canonical ensemble obtained from quantum Monte Carlo simulations. Second-order phase transitions are denoted by solid lines, whereas first-order transitions are denoted by dashed lines.

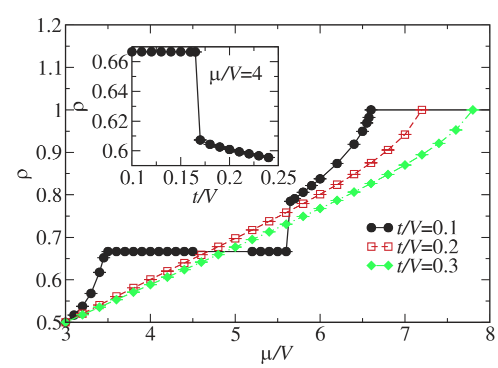

FIG. 3 (color online). Density of hard-core bosons on the triangular lattice as a function of μ along lines of constant values of t/V. The inset displays the jump in the density as a function of t for $\mu/V = 4$ at $t/V \approx 0.165$.

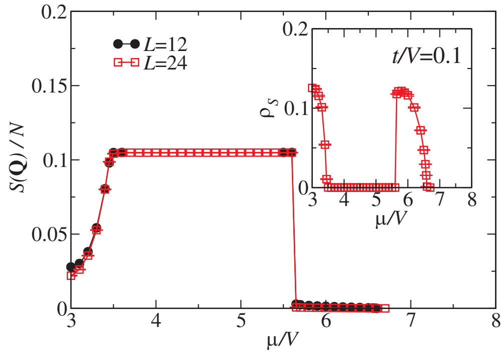

FIG. 4 (color online). Static structure factor $S(\mathbf{Q})$ for hard-core bosons on the triangular lattice as a function of μ along a line of constant $t/V = 0.1$. The inset shows the behavior of the superfluid density ρ_S.

A different situation exists for $\rho < 2/3$, since there is no symmetry around $\rho = 2/3$. Here, forming a domain wall would cost extra potential energy, and a supersolid phase can thus be stabilized. To demonstrate the existence of this supersolid even at half filling, we show the finite size scaling of ρ_S and $S(\mathbf{Q})$ in Fig. 6, both of which extrapolate to finite values. Intervening the solid phases at $1/3 < \rho < 2/3$ we hence find an extended supersolid phase, where both the superfluid density and the density structure factor take on finite values. Figure 7 shows ρ_S and $S(\mathbf{Q})$ as functions of t/V at half filling, indicating a continuous quantum phase transition from the supersolid to the superfluid at $t/V \approx 0.115$. We observe a kink in $\rho_S(t)$ near the transition point, marked by an arrow in Fig. 7. Away from half filling, the extend of the supersolid phase slightly increases, as shown in Fig. 2. Moreover, the kink in $\rho_S(t)$ at the supersolid-superfluid transition becomes more pronounced, being clearly visible for $\mu/V = 3.4$ in Fig. 8. Eventually, for $\mu/V > 3.95$, the supersolid phase ceases to be stable, giving rise to a direct first-order transition between the solid and the superfluid. This is reflected in discontinuities of both ρ_S and $S(\mathbf{Q})$ in Fig. 8, as well as in the density ρ (Fig. 3).

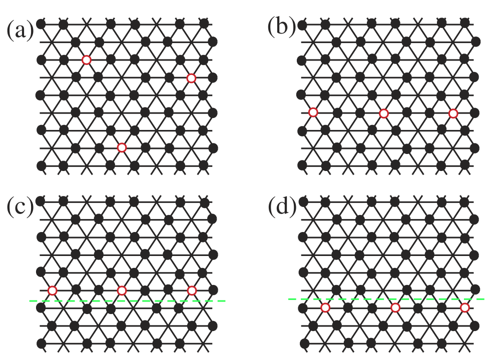

FIG. 5 (color online). The $\rho = 2/3$ solid doped with bosons. (a) Additional bosons (open circles) added on top of the solid. (b) Lining the bosons up costs no additional potential energy. (c) Shifting the lower half of the lattice introduces a domain wall (dashed line) at no cost, but now (d) the additional particles can hop freely across the domain wall, gaining additional kinetic energy.

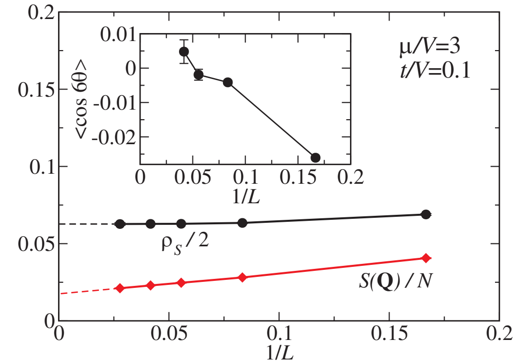

FIG. 6 (color online). Finite size scaling of the static structure factor $S(\mathbf{Q})$ and the superfluid density ρ_S for hard-core bosons on the triangular lattice at $t/V = 0.1$ and $\mu/V = 3$. Dashed lines are extrapolations to the infinite lattice. The inset shows the finite size scaling of the order parameter $\langle\cos(6\theta)\rangle$.

To summarize, we have demonstrated that an extended supersolid phase exists for hard-core bosons on the triangular lattice. This supersolid phase in the density regime $1/2 < \rho < 2/3$ emerges from a hugely degenerate disordered ground state of the frustrated classical model (in the $t = 0$ limit) when the quantum mechanical hopping is turned on. This illustrates an intriguing mechanism by which a quantum system can avoid frustration: in the low-density region, $\rho < 1/2$, a fraction $\rho - 1/3$ of the bosons delocalize and break the $U(1)$ gauge symmetry, forming a superfluid Bose condensate on top of the solid with density $\rho = 1/3$, that breaks translational symmetry, thus realizing a supersolid phase. An analogous picture holds for the supersoild emerging from the $2/3$ solid upon hole doping for $\rho > 1/2$. In order to characterize the density distribution inside the supersolid phase at $\rho = 1/2$, we consider the complex order parameter $me^{i\theta} = m_1 + m_2 e^{i4\pi/3} + m_3 e^{-i4\pi/3}$ in terms of the three sublattice densities $n_i = 1/2 + m_i$, $i = 1, 2, 3$. A value of $\langle\cos(6\theta)\rangle > 0$

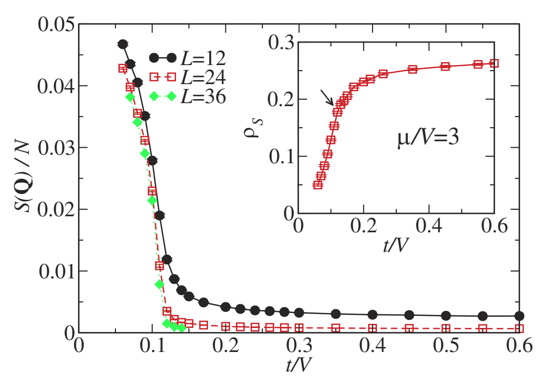

FIG. 7 (color online). Static structure factor $S(\mathbf{Q})$ for hard-core bosons on the triangular lattice as a function of t at half filling ($\mu/V = 3$). The inset shows the behavior of the superfluid density ρ_S with a kink at $t/V \approx 0.12$, indicated by an arrow.

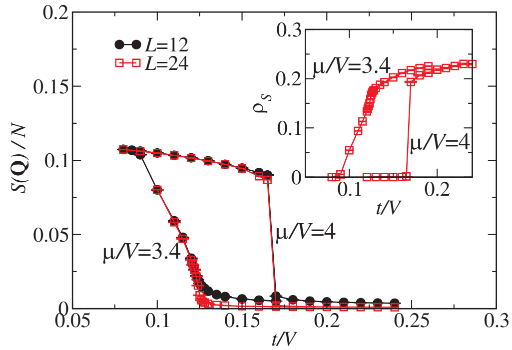

FIG. 8 (color online). Static structure factor $S(\mathbf{Q})$ for hard-core bosons on the triangular lattice as a function of t along lines of constant $\mu/V = 3.4$ and $\mu/V = 4$. The inset shows the superfluid density ρ_S, exhibiting a kink at $t/V \approx 0.125$ for $\mu/V = 3.4$.

indicates sublattice density orderings $(m_1, m_2, m_3) = (\pm 2m, \mp m, \mp m)$, whereas $\langle\cos(6\theta)\rangle < 0$ would correspond to a $(m, -m, 0)$ pattern [27]. From our simulations we find that $\langle\cos(6\theta)\rangle$ crosses over from negative to positive values upon increasing the system size, as seen in the inset of Fig. 6. This suggests that in the thermodynamic limit the supersolid at $\rho = 1/2$ marks a first-order transition between the low- and high-density supersolid states. It will be of interest to better characterize this quantum phase transition between different supersolid phases as a function of doping, as well as the thermal phase transitions.

The emergence of a supersolid on the triangular lattice is a variant of an order-by-disorder [28] mechanism, in which by the creation of a supersolid the degenerate disordered classical ground state is avoided in the quantum system. Since, in contrast to the square lattice, the realization of a supersolid on the triangular lattice does not require longer-ranged repulsion or hopping terms, nor a reduction of the on-site interaction [16], the triangular lattice offers the experimentally easiest possibility for realizing order-by-disorder phenomena and supersolid phases of ultracold atoms on optical lattices.

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Note added in proof.—Recently, we became aware of similar work concentrating on the supersolid phase at $\mu/V = 3$ [30–33]. While the authors of Ref. [30] argue for a $(\pm 2m, \mp m', \mp m')$ ordering pattern with $m' \neq m$, in Ref. [31] a $(m, -m, 0)$ pattern is proposed, whereas Ref. [32] provides further evidence for the first-order supersolid-supersolid transition at half filling.

[1] E. Kim and M. H. W. Chan, Nature (London) **427**, 225 (2004); Science **305**, 1941 (2004).
[2] A. Leggett, Science **305**, 1921 (2004); A. S. Moskvin, I. G. Bostrem, and A. S. Ovchinnikov, JETP Lett. **78**, 772 (2003).
[3] N. Prokof'ev and B. Svistunov, Phys. Rev. Lett. **94**, 155302 (2005).
[4] O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956); A. F. Andreev and I. M. Lifshitz, Sov. Phys. JETP **29**, 1107 (1969); G. Chester, Phys. Rev. A **2**, 256 (1970); A. J. Leggett, Phys. Rev. Lett. **25**, 1543 (1970).
[5] P. W. Anderson, *Basic Notions of Condensed Matter Physics* (Benjamin, New York, 1984).
[6] K. Góral, L. Santos, and M. Lewenstein, Phys. Rev. Lett. **88**, 170406 (2002).
[7] H. P. Büchler and G. Blatter, Phys. Rev. Lett. **91**, 130404 (2003).
[8] A. Griesmaier *et al.*, Phys. Rev. Lett. **94**, 160401 (2005).
[9] H. Matsuda and T. Tsuneto, Suppl. Prog. Theor. Phys. **46**, 411 (1970); W. J. Mullin, Phys. Rev. Lett. **26**, 611 (1971); K. S. Liu and M. E. Fisher, J. Low Temp. Phys. **10**, 655 (1973); E. Roddick and D. Stroud, Phys. Rev. B **48**, 16600 (1993); **51**, R8672 (1995); R. Micnas, S. Robaszkiewicz, and T. Kostyrko, *ibid.* **52**, 6863 (1995); E. S. Sorensen and E. Roddick, *ibid.* **53**, R8867 (1996).
[10] G. G. Batrouni *et al.*, Phys. Rev. Lett. **74**, 2527 (1995); R. T. Scalettar *et al.*, Phys. Rev. B **51**, 8467 (1995).
[11] E. Frey and L. Balents, Phys. Rev. B **55**, 1050 (1997).
[12] A. van Otterlo and K.-H. Wagenblast, Phys. Rev. Lett. **72**, 3598 (1994); A. van Otterlo *et al.*, Phys. Rev. B **52**, 16176 (1995).
[13] G. G. Batrouni and R. T. Scalettar, Phys. Rev. Lett. **84**, 1599 (2000); F. Hébert *et al.*, Phys. Rev. B **65**, 014513 (2002);
[14] M. Kohno and M. Takahashi, Phys. Rev. B **56**, 3212 (1997); A. Kuklov, N. Prokof'ev, and B. Svistunov, Phys. Rev. Lett. **93**, 230402 (2004).
[15] G. Schmid *et al.*, Phys. Rev. Lett. **88**, 167208 (2002).
[16] P. Sengupta *et al.*, Phys. Rev. Lett. **94**, 207202 (2005).
[17] G. Schmid, Ph.D. thesis, ETH Zürich, 2004.
[18] E. Burovski *et al.*, Phys. Rev. Lett. **94**, 165301 (2005).
[19] G. Schmid and M. Troyer, Phys. Rev. Lett. **93**, 067003 (2004).
[20] B. D. Metcalf, Phys. Lett. **45A**, 1 (1973).
[21] G. H. Wannier, Phys. Rev. **79**, 357 (1950).
[22] G. Murthy, D. Arovas, and A. Auerbach, Phys. Rev. B **55**, 3104 (1997).
[23] A. W. Sandvik, Phys. Rev. B **59**, R14157 (1999).
[24] O. F. Syljuåsen and A. W. Sandvik, Phys. Rev. E **66**, 046701 (2002); F. Alet, S. Wessel, and M. Troyer, Phys. Rev. E **71**, 036706 (2005).
[25] M. Boninsegni, J. Low Temp. Phys. **132**, 39 (2003).
[26] E. L. Pollock and D. M. Ceperley, Phys. Rev. B **36**, 8343 (1987).
[27] S. V. Isakov and R. Moessner, Phys. Rev. B **68**, 104409 (2003).
[28] J. Villain *et al.*, J. Phys. (Paris) **41**, 1263 (1980); C. L. Henley, Phys. Rev. Lett. **62**, 2056 (1989).
[29] M. Troyer *et al.*, Lect. Notes Comput. Sci. **1505**, 191 (1998); F. Alet *et al.*, J. Phys. Soc. Jpn. Suppl. **74**, 30 (2005).
[30] D. Heidarian and K. Damle, cond-mat/0505257.
[31] R. Melko *et al.*, cond-mat/0505258.
[32] M. Boninsegni and N. Prokof'ev, cond-mat/0507620.
[33] A. A. Burkov and L. Balents, cond-mat/0506457.