Melting of Bosonic Stripes

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We use quantum Monte Carlo simulations to determine the finite temperature phase diagram and to investigate the thermal and quantum melting of stripe phases in a two-dimensional hard-core boson model. At half filling and low temperatures the stripes melt at a first order transition. In the doped system, the melting transitions of the smectic phase at high temperatures and the superfluid smectic (supersolid) phase at low temperatures are either very weakly first order, or of second order with no clear indications for an intermediate nematic phase.

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Stripe phases of lattice models with broken rotational and translational symmetry can melt in two qualitatively different ways. One scenario is that both symmetries can be restored at a single first or second order transition, and the stripes melt directly into a normal fluid or superfluid phase. The other scenario is that first the translational symmetry is restored when the striped solid melts into a nematic (liquid crystal) phase with broken rotational symmetry. The rotational symmetry is then restored in a second melting transition of the nematic phase.

This quantum lattice problem shows similarities to the long standing-problem of the melting of a two dimensional crystal into a continuum model, where there is also either a first order melting or the Kosterlitz-Thouless-Halperin-Nelson-Young scenario of two Kosterlitz-Thouless transitions with an intervening hexactic phase [1]. Clear results for the classical version of this continuum problem were obtained only recently in a simple model of hard disks [2].

Current interest in quantum mechanical stripe phases and their melting stems from the experimental observation of stripes in some high-T_c superconductors [3] and from the questions whether and how they are related to the occurrence of high temperature superconductivity. Numerically, stripe phases have been found to be competitive ground states of t-J-like models [4,5]. Analytically some theories of high temperature superconductivity are closely linked to the existence of stripe and nematic phases [6]. Stripe phases exist also in non-superconducting compunds as, e.g., LSNiO [7] and have been found in the $\nu = 9/2, 11/2, 13/2, \ldots$ fractional quantum Hall systems [8].

While it is hard to study stripe phases directly in strongly correlated fermionic models, because of the negative sign problem of quantum Monte Carlo, we can more accurately investigate bosonic stripes using modern quantum Monte Carlo (QMC) algorithms [9–11]. Such bosonic models can appear as effective low energy models neglecting nodal quasiparticles [5,12]. Like the cuprates, these bosonic models show competition and in some models coexistence of superfluidity and charge order. In this Letter we focus on the simplest bosonic quantum model exhibiting stripe order and determine its finite temperature phase diagram. We carefully investigate its thermal and quantum melting transitions to address the question of how stripe melting occurs in a quantum model of bosonic stripes.

Stripe-ordered ground states have been found in the square lattice hard-core boson model with next nearest neighbor repulsions V_2 larger than half of the nearest neighbor repulsion $V_1/2$ [13–15]. Since the stripe phase at finite nearest neighbor repulsion V_1 connects continuously with the stripe phase at $V_1 = 0$ [15] we here set $V_1 = 0$ and focus on the simplest model containing only a next nearest neighbor interaction:

$$H = -t\sum_{\langle \mathbf{i},\mathbf{j}\rangle}(a_{\mathbf{i}}^{\dagger}a_{\mathbf{j}} + a_{\mathbf{j}}^{\dagger}a_{\mathbf{i}}) + V_2\sum_{\langle\langle \mathbf{i},\mathbf{j}\rangle\rangle} n_{\mathbf{i}}n_{\mathbf{j}} - \mu\sum_{\mathbf{i}} n_{\mathbf{i}}, \quad (1)$$

where $a_{\mathbf{i}}^{\dagger}$ ($a_{\mathbf{i}}$) is the creation (annihilation) operator for hard-core bosons, $n_{\mathbf{i}} = a_{\mathbf{i}}^{\dagger}a_{\mathbf{i}}$ is the number operator, $V_2 \geq 0$ are the next nearest neighbor Coulomb repulsions, and μ is the chemical potential.

In Fig. 1 we review the ground-state phase diagram of this model which was previously studied by mean-field calculations, renormalization group approaches, and local-update QMC simulations [13–15]. At half filling (density $\rho = 1/2$ at $\mu = 2V_2$) the ground state is a smectic for small values of t/V_2 and the quantum melting transition at low temperatures was found to be of first order (translation symmetry is broken only in one dimension, perpendicular to the stripes; hence this phase is a smectic). Doping this smectic stripe crystal a stable "supersolid" phase with coexisting stripe order and superfluidity was found, in which the vacancies doped into the stripes form a superfluid.

Before going into details we summarize our key results by presenting the finite temperature phase diagrams along the lines indicated in the ground state phase diagram Fig. 1. At half filling with density $\rho = 1/2$ we find that stripe order and superfluidity compete at low temperatures, resulting in a strong first order phase transition between the two phases [see Fig. 2(a)]. At higher tem-

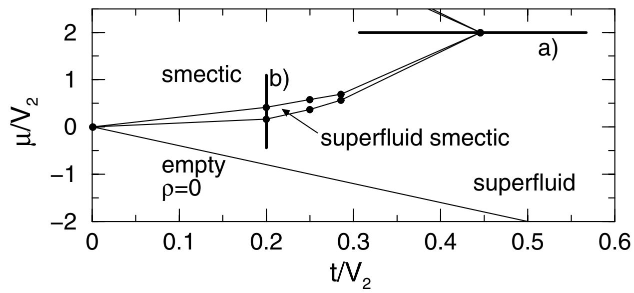

FIG. 1. Ground-state phase diagram of the hard-core boson Hubbard model Eq. (1) as a function of t/V_2 and μ/V_2. Because of particle-hole symmetry, the phase diagram is symmetric around the half filling line (density $\rho = 1/2$ at $\mu = 2V_2$) and the lower half is shown. The thick lines (*a*) and (*b*) indicate the cuts along which we show the finite-temperature phase diagrams in Fig. 2.

peratures the stripes melt to a normal fluid phase. The order of that transition changes from weak first order to second order as $t/V_2 \to 0$. In contrast to half filling, the smectic stripe order and superfluidity can coexist when the stripes are doped away from half filling [Fig. 2(b)], but the critical temperature of either order is suppressed by the other one. We find that the superfluid smectic (supersolid) phase behaves as a dilute gas of free hard-core bosons, with density $|\rho - 1/2|$ on an anisotropic smectic stripe background. The phase transitions away from half filling are all either very weakly first order or of second order. Rotational and translational symmetry breaking occur, within our accuracy, at the same point, and no nematic phase was observed.

Our results were obtained by a directed loop quantum Monte Carlo simulation in the stochastic series expansion representation [9]. The simulations were performed in the grand canonical ensemble and do not suffer from any systematic errors apart from finite size effects. Stripe order is measured by the order parameter

$$O_S = S_n(\pi, 0) + S_n(0, \pi), \tag{2}$$

where $S_n(k_x, k_y)$ is the charge structure factor at the wave vector (k_x, k_y). To investigate a nematic phase, we have to look for rotational symmetry breaking in the kinetic energy or in the local charge correlations, using as order parameters

$$O_k = \frac{1}{V}\sum_{(x,y)} a^\dagger_{(x,y)}a_{(x+1,y)} - a^\dagger_{(x,y)}a_{(x,y+1)} + \text{H.c.} \tag{3}$$

or alternatively

$$O_N = \sum_{(x,y)} n_{(x,y)}n_{(x+1,y)} - n_{(x,y)}n_{(x,y+1)}, \tag{4}$$

where $n_{(x,y)} = a^\dagger_{(x,y)}a_{(x,y)}$ is the boson number operator at lattice site (x, y) and H.c. denotes the Hermitian conjugate. The extent of the superfluid phase is determined by measuring the superfluid (number) density $\rho_s = mT\langle W^2\rangle$, where W is the winding number in one of the directions and m is the mass of a boson. ρ_s is finite in the superfluid phase and jumps to zero from a universal value $\frac{2}{\pi}mT_c$ at the Kosterlitz-Thouless transition.

We now discuss the phase diagrams and the nature of the phase transitions in more detail, starting with the *half filled* system at $\mu = 2V_2$, where a first order quantum phase transition is found at $V_2/t = 2.24 \pm 0.03$, improving the previous estimate of Ref. [15]. When raising the temperature we find that the transition remains of first order as the histograms for both the stripe order parameter O_S and the rotational symmetry breaking order parameter O_N show two clearly separated peaks corresponding to the two coexisting phases (Fig. 3). These two peaks survive finite size extrapolations from simulations on system sizes $L = 8$, 16, and 32 and indicate a single strong first order transition up to at least $T/t = 2/3$ [from point (D) to (B) in Fig. 2(a)].

Measuring the superfluid density ρ_s at the coexistence line for configurations in the fluid phase (determined by their value of O_S), we find that at low temperatures $T/t \leq 1/2$ [point (C)] the stripes melt into a superfluid, while at $T/t \geq 2/3$ [point (B)], they melt into a normal fluid—

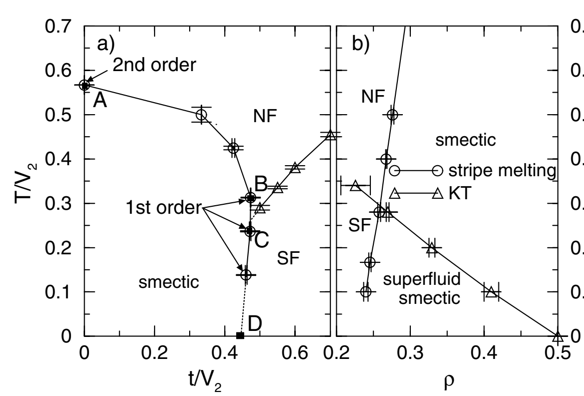

FIG. 2. (a) Finite temperature phase diagram as a function of t/V_2 of the half filled model and (b) as a function of the density ρ along the respective lines of Fig. 1. The normal fluid and superfluid phases are denoted by the symbols NF and SF.

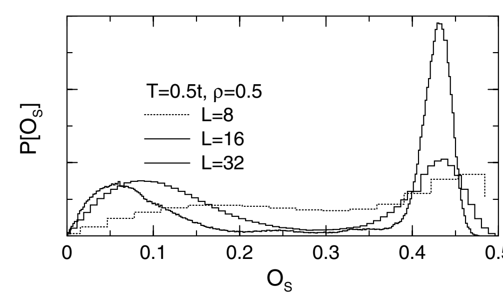

FIG. 3. Histograms of the stripe order parameter O_S clearly show the double-peak structure of a first order transition which gets more pronounced as the system size is increased.

hence there is a tricritcal point in the range $1/2 < T/t < 2/3$ (between points B and C), where the Kosterlitz-Thouless phase transition of the superfluid turns into a first order transition.

At higher temperatures and larger repulsion V_2 it becomes harder to determine the order of the phase transition. At $V_2 = 3t$ no double-peak structure could be seen in the histograms for lattice sizes up to $L = 32$, and the transition is thus either second order or a very weak first order transition. In the limit of infinite repulsion V_2 the lattice decouples into two sublattices, each of which is equivalent to an Ising antiferromagnet with a second order melting transition. We thus explore the possibility of a second order transition, where the fourth order cumulant ratios $C_4 = 1 - \langle O^4\rangle/3\langle O^2\rangle^2$ have a size independent value at the transition point. Figure 4 indeed shows a crossing of the Binder cumulants of different system sizes in a single point, which is an indication for second order transition. Both the fourth order cumulant ratios for both O_N and O_S cross at the same temperature within the accuracy of our results, indicating that translational symmetry breaking (measured by O_S) and rotational symmetry breaking (measured by O_N) happen at the same or at very close temperatures, without evidence for an intervening nematic phase.

The phase diagram of the *doped system* away from half filling shows an additional supersolid phase where the vacancies doped into the stripes form a superfluid smectic with broken translational and rotational symmetry as well as a finite superfluid density. Since the rotational symmetry is spontaneously broken in the smectic phase, the superfluid becomes anisotropic. The superfluid density is replaced by the geometric mean $\rho_s = \sqrt{\rho_{s,||}\rho_{s,\perp}}$, where the superfluid densities parallel ($\rho_{s,||}$) and perpendicular ($\rho_{s,\perp}$) to the stripe order were measured for each configuration from the winding numbers in either the x or the y direction depending on whether $S_n(0,\pi)$ was larger or smaller than $S_n(\pi, 0)$. Care was taken that the anisotropy did not become too large to introduce systematic errors [16].

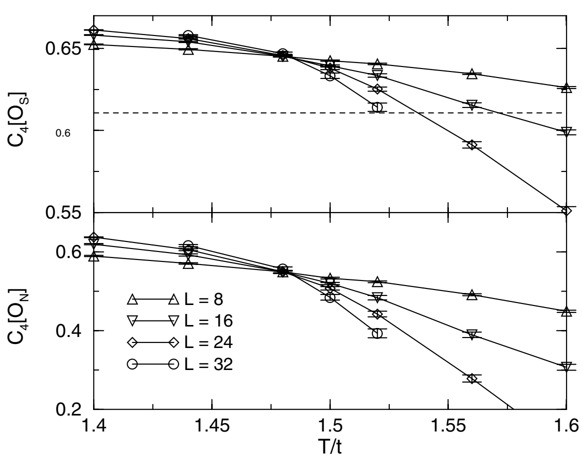

FIG. 4. Fourth order cumulants for O_S and O_N as a function of the temperature ($V_1 = 0$, $V_2 = 3t$). The dashed horizontal line shows the critical value for a second order transition in the Ising universality class. The crossing point of the fourth order cumulant ratios for O_S is not consistent with this value.

Although superfluidity coexists with smectic order, it is strongly suppressed and T_c and ρ_s vanish linearly as half filling is approached. Using $m_{||} = 1/2t$ and $m_\perp = \frac{1}{2t^2/(4V_2)}$ as the boson masses parallel and perpendicular to the stripes, respectively, we obtain $\rho_s = (0.78 \pm 0.07)2|\rho - \frac{1}{2}|$ consistent with the value obtained previously for a dilute gas of bosons [17]. The superfluid smectic (supersolid) phase can thus be viewed as a gas of dilute bosons with density $2|\rho - 1/2|$. These bosons are the interstitials (at $\rho > 1/2$) or vacancies (at $\rho < 1/2$) of the doped stripe phase.

We repeat a similar procedure as at half filling to determine the nature of the phase transitions. In contrast to the half filled case, the doped case of the nearest neighbor model [18], and previous simulations of the current model by local update methods on small lattices [15] we find no evidence for a first order transition. Instead we find the smooth behavior shown in Fig. 5, which is in agreement with analytical considerations using mean-field and spin-wave analysis [13] or renormalization group calculations [14]. We again determine the critical points for rotational and translational symmetry breaking at a temperature $T = t/6$ and a coupling $V_2/t = 5$, using both Binder cumulant ratios for O_S and O_N, and the maximum of the susceptibility associated with O_k for our estimate $\rho_c = 0.2468 \pm 0.0025$. Again, we find agreement—within the error bars—of the critical points for rotational and translational symmetry breaking, and no indication for a nematic phase.

Finally we want to discuss our results in view of the three possibilities for the nature of the melting transitions of (i) a first order transition, (ii) a single second order transition, or (iii) two separate second order transitions. Close to half filling and at low temperatures we have very clear evidence for a single first order transition. The

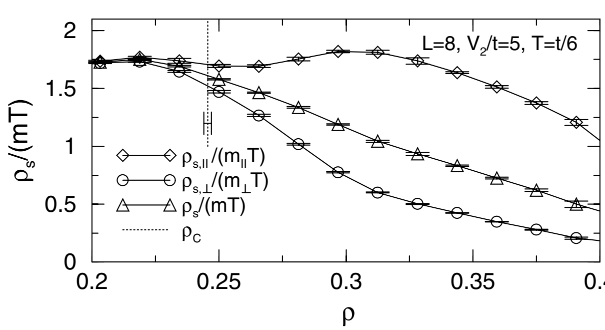

FIG. 5. Superfluid density parallel ($\rho_{s,||}$) and perpendicular ($\rho_{s,\perp}$) to the stripes for $L = 8$, $V_2/t = 5$, and $T = t/6$.

results for thermal melting at higher temperatures and for the doping-driven melting at low temperatures are not as clear-cut. While a very weak first order transition is always possible, it is more likely that we have second order transitions, especially in view of the fact that in the limit $t/V_2 \to \infty$ there will be a second order transition in the Ising universality class. One way to distinguish between the scenarios (ii) of one single transition or (iii) of two second order transitions with an intervening nematic phase is that in the latter case both transitions should be in the Ising universality class since they each break a Z_2 symmetry. At the transition we would thus expect that the Binder cumulant ratios at T_c take on the value $C_4 = 0.610\,690\,0(1)$ [19]. The fact that our results for the cumulant ratio of O_S are close but not identical to this universal value for an Ising transition rather indicates secnario (ii), a single second order transition in a different universality class. In the doped system our data both for the cumulant ratios and the scaling of the susceptibility of O_k are actually closer to the three dimensional XY universality class predicted by Ref. [14] than the Ising universality class. More extensive simulations on larger systems, using newly developed flat histogram methods for quantum systems [20] will be needed to more accurately determine the universality class of this phase transition.

Our results have shown that the simplest bosonic model already captures the physics of the coexistence between solid and superfluid order. A striped supersolid phase with coexisting stripe order and superfluidity is stable at finite temperature and behaves as a dilute gas of hard-core bosons on an anisotropic background. In the context of high temperature superconductivity it will be of interest, when more powerful computers become available, to extend the current investigation to more realistic models with stripes at $1/8$ doping. These stripes will be described by effective models with longer ranged interactions, which could be obtained from density matrix renormalization group or contractor renormalization calculations, extending the work in Ref. [12].

While the exact order and universality class of the melting transition are hard to determine—which is not surprising given the difficulties known from the similar classical problem in the continuum—our results are clear with respect to the existence of a nematic phase. Such a phase must be restricted to a very narrow temperature and doping regime, smaller than the resolution of our simulations and does not seem to be a generic phase in bosonic models like Eq. (1). It might be possible to stabilize a nematic phase with additional terms in the Hamiltonian. One suggestion [21] is to add a term proportional to the square of the nematic order parameter $-VO_k^2$, to stabilize a nematic phase. This term gives two contributions: a nearest neighbor repulsion $2V\sum_{\langle \mathbf{i},\mathbf{j}\rangle} n_{\mathbf{i}} n_{\mathbf{j}}$ and an additional next nearest neighbor hopping term $V\sum_{\langle\langle i,j\rangle\rangle}(a_{\mathbf{i}}^\dagger a_{\mathbf{j}} + a_{\mathbf{j}}^\dagger a_{\mathbf{i}})$. The latter, *frustrated hopping* term, which unfortunately causes a negative sign problem for quantum Monte Carlo simulations, might be important for the stability of an extended nematic phase. It is interesting to compare this model with the related frustrated Heisenberg model on a square lattice. In that model, which also exhibits translational and rotational symmetry breaking in the ground state, it is at present controversial whether these symmetry broken phases extend to finite temperatures [22,23].

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