On the 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-Thouless-Halperin-Nelson-Young (KTHNY) 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 question 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]. While it is hard to study stripe phases 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 algorithms [7, 8]. Such bosonic models can appear as effective low energy models neglecting nodal quasiparticles [9, 10]. 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. The particular hard-core boson Hubbard Hamiltonian we study on a two-dimensional square lattice is

$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + V_2 \sum_i n_i n_j - \mu \sum_i n_i, \quad (1)$$

where $a_i^\dagger$ ($a_i$) is the creation (annihilation) operator for hard-core bosons, $n_i = a_i^\dagger a_i$ the number operator, $V_2 \geq 0$ the next nearest neighbor Coulomb repulsions and $\mu$ the chemical potential. The Hamiltonian (1) is equivalent to an anisotropic spin-$1/2$ model with a nearest neighbor XY-like interaction $J_{xy} = 2t$ and next nearest neighbor Ising interaction $J'_z = V_2$ in a magnetic field $h = 2V_2 - \mu$.

In Fig. 1 we review the ground-state phase diagram of this model which was previously studied by mean-field, renormalization group and local-update quantum Monte Carlo simulations [10, 11, 12]. At half filling (density $\rho = 1/2$ at $\mu = 2V_2$) the ground state is a smectic for $t/V_2 < 0.446 \pm 0.006$ 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 (see Fig. 2b) we find that the transition between smectic and superfluid is of first order at all temperatures. At higher temperatures the transition between smectic and normal fluid is of first order at all temperatures. At half filling (see Fig. 2a) we find that the transition remains of first order as $t/V_2 \rightarrow 0$. In the doped system (see Fig. 2b) coexistence between the smectic phase and superfluidity can be observed at low temperatures around half filling. Here the phase transitions are all either very weakly first order or of second order. Rotational and translational symmetry breaking occur, within the accuracy of our simulations, at the same point.

To determine the finite-temperature phase diagram we have used quantum Monte Carlo simulations, employing a directed loop quantum Monte Carlo algorithm in the in the stochastic series expansion (SSE) representation 7. The simulations were performed in the grand canonical ensemble and do not suffer from any systematic errors apart from finite size effects. In contrast to the loop algorithm 3 the directed loop algorithm remains effective away from half filling where the loop algorithm slows down exponentially.

We determine stripe order by measuring the order parameter

$$O_s = S_n(\pi, 0) + S_n(0, \pi)$$

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

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

or alternatively

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

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

$$\rho_s = n T \langle W^2 \rangle \quad (5)$$

where $W$ is the winding number in one of the directions and $m$ the mass of a boson. $\rho_s$ is finite in the superfluid phase and jumps to zero from a universal value $2\pi m T_c$ 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 was found at $V_2/t = 2.24 \pm 0.03$, improving the previous estimate 12. When raising the temperature we find that the transition remains of first order as the histograms for the two 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 (see Fig. 3). Careful finite size scaling of the peak distances on system sizes $L = 8$ up to $L = 32$ show that the two peaks stay separate as expected for a first order transition and do not merge as in a second order one. For both order parameters we find the same phase transition line, confirming a melting in a single strong first order transition up to at least $T/t = 2/3$ [from point (D) to (B) in Fig. 2b].
To investigate whether the stripes melt into a superfluid or normal fluid we measure the superfluid density \( \rho_s \) at the coexistence line for configurations in the fluid phase (determined by their value of \( O_S \)). At a temperature \( T/t = 2/3 \) [point (B)], \( \rho_s \) drops below the universal jump value \( 2\pi mT \) as a function of system size \( L \) and will thus scale to zero in the infinite system. Hence the transition at this temperature is of first order to a normal fluid phase \([13]\). There is thus a tricritical point between points B and C where the Kosterlitz-Thouless phase transition of the superfluid becomes first order.

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 sub-lattices, 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. For a second order transition the 4-th 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, which can be found as the crossing points of the cumulants for different system sizes. Our results (see Fig. 4) show that we indeed observe such crossings, which is an indication for second order transition. Both the 4-th 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.

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 and Eq. (5) for the superfluid density needs to be modified. The geometric mean of the superfluid densities perpendicular and parallel to the stripes \( \rho_s = \sqrt{\rho_{s,||} \cdot \rho_{s,\perp}} \) is the quantity exhibiting the universal jump at the Kosterlitz-Thouless transition and was used in the determination of the phase transition. Care was taken that the anisotropy did not become too large to introduce systematic errors as pointed out by Prokof’ev and Svistunov [14]. 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 \( x \) or \( y \) direction depending on whether \( S_n(0, \pi) \) was larger or smaller than \( S_n(\pi, 0) \).

Although superfluidity coexists with smectic order, it is strongly suppressed and \( T_c \) and \( \rho_s \) vanish linearly as half filling is approached. Using \( m_{||} = 1/2t \) and \( m_{\perp} = \frac{1}{2\pi/(\sqrt{V_2})} \) as the boson masses parallel and perpendicular to the stripes, respectively, we obtain \( \rho_s = (0.78 \pm 0.07)t \rho - 1/2 \) consistent with the value obtained previously for a dilute gas of bosons [15].

In order to investigate the nature of the doping-driven melting of the smectic phase we repeat a similar procedure as at half filling. In contrast to the half filled case, with a clear jump in the values of \( O_S \) and \( O_N \) at the phase transition, or in the doped case of the nearest neighbor model with a jump in density \( \rho \) at the doping-driven melting transition [16], no such jump or double-peak structure was observed here. We checked the order parameters \( O_S \), \( O_N \), \( O_{4s} \), and the density \( \rho \) in systems with size up to \( L = 48 \). Repeating the simulations of Ref. [12], where a local update algorithm was used instead of our nonlocal algorithm we cannot reproduce the
jump in the superfluid density seen there. Instead we find the smooth behavior shown in Fig. 5 for the same system, which is also in agreement with analytical considerations using mean-field and spin-wave analysis [10] or renormalization group calculations [11]. Since our results are well converged and do not suffer from any systematic error, we believe the differences to be due to the method used to calculate the superfluid densities in Ref. [12].

At $T = t/6$ we checked whether rotational and translational symmetry breaking occur at the same critical density by comparing estimates obtained using Binder cumulant ratios for $O_S$ and $O_N$ as well as a determination of the critical point from the maxima of the susceptibility associated with $O_k$. The estimates agree within the error bars: $\rho_c = 0.2468 \pm 0.0025$ at $T = t/6$.

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 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 $C_4 = 0.6106900(1)$ [17]. 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 scenario (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. [17] than the Ising universality class. More extensive simulations on larger systems, using newly developed flat histogram methods for quantum systems [18] will be needed to more accurately determine the universality class of this phase transition.

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 interesting also 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. It might be possible to stabilize a nematic phase with additional terms in the Hamiltonian. One suggestion [19] is to add a term proportional to the square of the nematic order parameter $-V O^2_k$, to stabilize a nematic phase. This term gives two contributions: a nearest neighbor repulsion $2V \sum_{\langle i,j \rangle} a_i a_j$ and an additional next nearest neighbor hopping term $V \sum_{\langle\langle i,j \rangle\rangle} (a_i^\dagger a_j + a_j^\dagger a_i)$. These frustrating terms, the second of 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 which however exhibits translational and rotational symmetry breaking only in the ground state at $T = 0$ [20].

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