Flux lattice melting and depinning in the weakly frustrated two-dimensional XY model

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Monte Carlo simulations of the frustrated two-dimensional (2D) XY model were carried out at small commensurate values of the frustration f. For $f = 1/30$ a single transition was observed at which phase coherence (finite helicity modulus) and vortex lattice orientational order vanish together. For $f = 1/56$ a new phase in which phase coherence is absent but orientational order persists was observed. Where comparison is possible, the results are in detailed agreement with the behavior of the lattice Coulomb gas model of vortices. It is argued that the helicity modulus of the frustrated 2D XY model vanishes for any finite temperature in the limit of weak frustration f.

Motivated by high-temperature superconductors, there has been renewed interest recently in the nature of phase transitions, if any, in strongly type II two-dimensional (2D) superconductors in applied magnetic fields.[1] One approach to the 2D problem in the infinite κ limit is provided by the lowest Landau level approximation to Ginzburg-Landau theory, where a truncated basis consisting only of states in the lowest Landau level of linearized Ginzburg-Landau theory is retained.[2] First order melting transitions have been observed in Monte Carlo simulations using this approach,[3] although no transition was observed in simulations on a sphere.[4] An alternative discretization procedure places Ginzburg-Landau functional on a lattice, usually by use of *phase only* models such as frustrated XY or Villain models. Here fluctuations in the amplitude of the superconducting order parameter are neglected, which is a reasonable approximation far from the critical temperature. In the XY and Villain models compactness (equivalence of states whose local superfluid phases differ by multiples of 2π) has been imposed in different ways.

The interaction potential of the Villain model has very special features. The model shows a separation of vortex and spin wave degrees of freedom; namely, after duality transformation, the partition sum factorizes into a product of spin wave (Gaussian) fluctuations and 2D lattice Coulomb gas components.[5] The lattice Coulomb gas amounts to a 2D "lattice London model" for the vortex state. It was on the basis of the continuum Coulomb gas model that Huberman and Doniach[6] and Fisher[7] discussed the vortex lattice melting transition in 2D superconductors. Here Kosterlitz-Thouless dislocation mediated melting theory[8,9] leads to a melting temperature estimate which is independent of vortex density. However, in a series of papers Moore,[10] has implicitly questioned the validity of the London model, and argued that the lower critical dimension for superconductivity is in fact $d = 4$.

The question naturally arises whether the phase only discretization of Ginzburg-Landau theory provided by the Villain model is fully equivalent to other discretization schemes. If it were not, then the validity of conclusions based on the Coulomb gas (London) model would be in doubt. For example, in the alternative discretization provided by the XY model, the separation of vortex and spin-wave degrees of freedom is not complete. Thus the London model is not strictly valid even for the vortex contribution to the thermodynamics. Both the lattice London and XY models have been extensively[11] used in studies of vortex lattice melting, and it is essential to know if they indeed share the same continuum limit.

In a recent Letter[12] Franz and Teitel reported very detailed Monte Carlo simulations of the lattice Coulomb gas (LCG) in two dimensions. While the discreteness of the lattice is expected to become unimportant in the dilute limit, these authors found that the "continuum limit" is subtle, and only reached for surprisingly small values of the density (denoted f). In sufficiently dilute systems, a "depinning" or "floating" phase transition occurs from a low temperature phase with long range translational order (LRTO) to a phase with algebraic order, followed by a first order 2D melting transition to a disordered phase. For dense systems, the phase with algebraic order is absent, i.e. depinning and melting transitions coincide. The existence of a phase with LRTO is an artifact of pinning in the lattice model because there is a finite energy cost for displacing a vortex in the ground state configuration. The appearance of a phase with algebraic order signals the onset of the continuum limit.

The transition temperature T_p at which LRTO disappears vanishes linearly in f. The 2D melting temperature, where algebraic order disappears, is independent of density as anticipated from 2D melting theory. The linear dependence of T_p on density in the dilute Coulomb gas can be established analytically[13]. The 2D *harmonic* Coulomb solid on a lattice can be mapped to a dislocation (vector plasma) problem, which has a continuous Kosterlitz-Thouless-Halperin-Nelson[8,9] unbinding transition, provided that the core energy for a dislocation is sufficiently large. In the dilute limit the core energy can be shown to grow as $\log(1/f)$ so that this condition is always satisfied. In the low temperature phase displacement fluctuations of the Coulomb solid are screened which permits LRTO even in 2D.

In this paper we report the results of a Monte Carlo study of the 2D XY model in the limit of weak commensurate frustration ($f = 1/q$, q = integer) with periodic boundary conditions. To avoid biasing the vortex system towards hexagonal order, we choose a square background grid. The 2D XY model is:

$$H = -\sum_{\langle i,j\rangle} \cos(\theta_i - \theta_j - A_{ij}) \quad (1)$$

where θ_i is the phase of the superconducting order parameter defined on an $L \times L$ square lattice of points labeled by i. The link field A_{ij} (line integral of the vector potential between nearest neighbor lattice sites i and j) satisfies $\sum A_{ij} = 2\pi\Phi/\Phi_0 \equiv 2\pi f$. The sum is taken counter clockwise around a plaquette. The magnetic flux per plaquette Φ is uniform which effectively imposes the infinite κ limit. Φ_0 is the flux quantum, and f is the frustration. The local vorticity $\nu(\mathbf{R})$ takes values $0, \pm 1$ and is defined via $\sum \mathrm{mod}(\theta_i - \theta_j - A_{ij}) = 2\pi(f - \nu)$ where the sum is around the plaquette $\mathbf{R}$[14]. $\mathrm{mod}(x)$ adds integer multiples of 2π to x to bring it into the range $(-\pi, \pi]$. With periodic or anti-periodic boundary conditions the total vorticity is constrained to equal the total applied flux; i.e the plaquette sum $\sum_{\mathbf{R}} \nu(\mathbf{R}) = L^2 f$.

The ground state spin configurations of the XY model in rational ($f = p/q$) magnetic fields change in a highly non-trivial way with p and q and have been the subject of a large literature[15]. We have succeeded in finding ground states for $f = 1/30$ and $f = 1/56$ appropriate to this study by slow cooling of $q \times q$ unit cells, using periodic boundary conditions for $f = 1/30$ and mixed periodic and anti-periodic conditions for $f = 1/56$. The vortex lattice is nearly triangular in these ground states as shown in Fig. 1. However, strictly speaking these states have only two-fold symmetry. Near hexagonal symmetry is associated with extra stability of these ground states.

At finite temperatures we measure the helicity modulus and six-fold orientational order parameter. The helicity modulus, Υ, is equivalent to the superfluid density[16] and is a measure of long range phase coherence. It is defined as the sensitivity of the free energy to a twist in the boundary condition along a particular direction via

$$\Upsilon = \frac{1}{L^2}\frac{\partial^2 F}{\partial \delta^2}\Big|_{\delta=0} \quad (2)$$

where δ is the twist angle.[17] Note that, for periodic boundary conditions, Υ measures the free energy shift

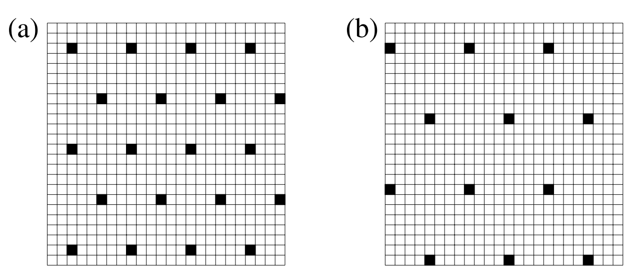

FIG. 1. The configuration of vortices in the ground states for (a) $f = 1/30$, and (b) $f = 1/56$. For convenience only system sizes 24×24 are shown.

in the presence of a flux loop of strength δ about the interior of the torus. The helicity modulus is therefore a *gauge invariant* response.

In the continuum, a 2D solid has finite orientational order below it's melting temperature. The six-fold orientational order parameter is,

$$\varphi_6 = \frac{1}{(fL^2)^2}\langle \sum_{k,l} \exp[6\imath(\phi_k - \phi_l)]\rangle \quad (3)$$

where ϕ_k is the angle between a fixed direction in the XY plane and the direction of the bond between vortex k and its nearest neighbor. $\varphi_6 = 1$ for a perfect triangular lattice.

We used a heat bath method for the simulations heating up slowly from the ground states. For $f = 1/30$ we simulated systems with linear dimension $L = 60 and 90$, and for $f = 1/56$ we simulated systems of size $L = 56$ and 112. Before computing any averages the system was carefully thermalized at each temperature discarding $120,000 - 680,000$ Monte Carlo sweeps (MCS) over the entire lattice. From these thermalized states we computed four averages using $20,000$ MCS, from which the final averages were calculated and the error estimated from the standard deviation. For the simulations we used several months of CPU time on a Hewlett Packarard model HP7000 workstation. The task is more difficult than simulations of the LCG, since there are $1/f$ times as many degrees of freedom involved in the updating algorithm. Furthermore, the system sizes accessible are restricted by the fact that the ground states are only periodic on at best $q \times q$ systems.[15] For these reasons careful finite size scaling was impractical.

A second important difference between XY and LCG models from the point of view of Monte Carlo simulation is the presence of energy barriers to the motion of isolated vortices in the XY model. To move a vortex through one lattice constant requires finite motion of spins in the vicinity of the vortex. This energy barrier has been estimated to be $E_p \sim 0.2$,[18] and plays an important role in the physics of Josephson junction arrays. The barrier means that equilibration times become long at temperatures $T \ll E_p$. Surprisingly, and for reasons not completely clear to us, this problem was less severe than expected, and the system equilibrates even at temperatures of order $0.1E_p$, as evidenced by our ability to find ground states by cooling. Further details of the Monte Carlo procedure and additional results from these investigations will be presented elsewhere.[19]

Fig. 2 shows the computed curves for the Υ and φ_6. For $f = 1/30$ orientational order and long range phase coherence remain finite up to $T_p \approx 0.045$, where they both drop rapidly to values around zero. These data are consistent with a single T_p at which both order parameters vanish. For $f = 1/56$ the helicity modulus vanishes at $T_p \approx 0.03$. At this temperature the orientational order also falls, but to a clearly finite value. Orientational order persists up to $T_m \approx 0.05$. The finite size effect is small. Note that the melting temperature has not changed significantly between $f = 1/30$ and $f = 1/56$.

As discussed above, to fully characterize the three

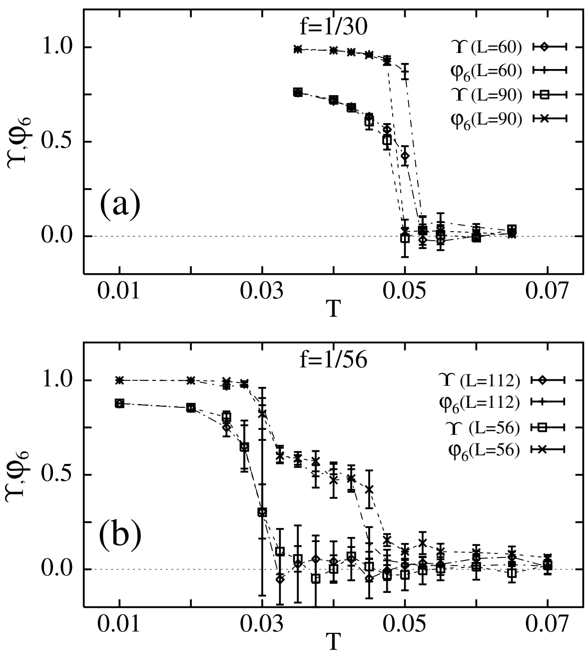

FIG. 2. Orientational order and helicity modulus for (a) $f = 1/30, L = 60$ and $L = 90$, (b) $f = 1/56, L = 56$ and $L = 112$. Errorbars correspond to $\pm$ one standard deviation. Lines are guides to the eye.

phases and extract exponents for the two phase transitions is a difficult task within the framework of XY model simulations. However, it is possible to identify the phases with reasonable certainty by analogy with the LCG, and by qualitative features of the structure function. The results for $f = 1/56$ clearly show the existence of two distinct phase transitions. The first one at T_p is associated with the depinning of the vortex lattice from the underlying mesh. The helicity modulus vanishes at the depinning transition, but orientational order persists, consistent with the idea that the vortices form a lattice with at least algebraic translational order.

These results should be compared with Franz and Teitel's[12] LCG simulations on a square lattice, who found that $T_p < T_m$ for $f \lesssim 1/30$ Their $f = 1/60$ results are equivalent, in our units, to $T_p = 0.028$ and $T_m = 0.047$. Comparing Fig. 2 we see there is semi-quantitative agreement between the behavior of the LCG model and the XY model. In particular comparison with Fig. 1 of ref. [12] shows that there is a striking similarity between the behavior of the inverse dielectric function of the LCG and the helicity modulus of XY model. While the connection between $\epsilon^{-1}(T)$ and $\Upsilon(T)$ can be rigorously established only for the Villain model,[5] the close analogy between these two quantities is evident.

This interpretation is supported by the behavior of the vortex lattice structure function,

$$S(\mathbf{q}) = \frac{1}{L^2} \sum_{\mathbf{R}_i} \exp[\imath \mathbf{q} \cdot \mathbf{R}_i] \langle \nu(\mathbf{R}_i) \nu(0) \rangle. \quad (4)$$

Fig. 3 shows $S(\mathbf{q})$ for $f = 1/56$ for temperatures $T = 0.02, 0.04$ and 0.06 corresponding to the three phases of Fig. 2.b. In the low temperature phase the Bragg peaks are well defined out to high orders. In the intermediate temperature phase, the Bragg peak structure is still present, but the intensity of each peak is much weaker, and falls quickly with order. The near hexagonal symmetry remains clear, compatible with algebraic order. In the high temperature phase the Bragg peak structure is absent and only the circular symmetry characteristic of a liquid is present.

Long range phase coherence disappears at the depinning transition, leading directly to the conclusion that the unpinned ideal vortex lattice with algebraic order has no long range phase coherence and is not superfluid.[20,21] Moreover, on the basis of the close analogy between the LCG and frustrated XY models, T_p is expected to vanish linearly in the limit of small f and thus the superfluid

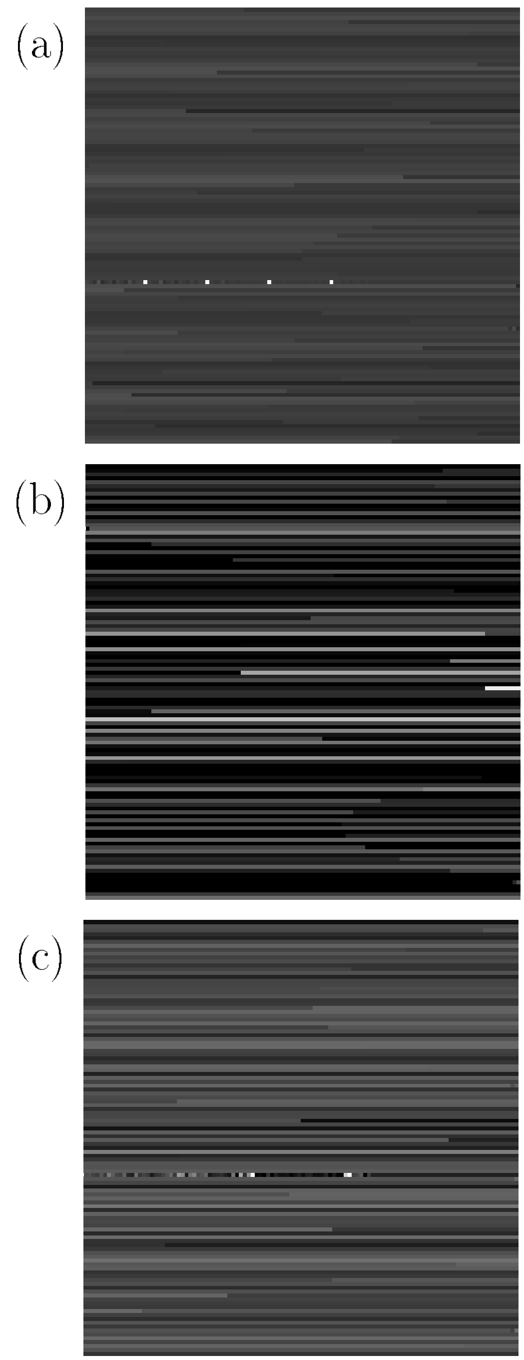

FIG. 3. Vortex structure function in the square lattice Brillouin zone for $f = 1/56$ and $L = 112$ at temperatures (a) $T = 0.02$, (b) $T = 0.04$ and (c) $T = 0.06$.

stiffness of the XY model vanishes in this limit. This is remarkable because, as is well known, the helicity modulus of the *unfrustrated* XY model is finite up to the vortex unbinding transition[8] at $T_c = 0.9$.[22] Here the transition mechanism is the unbinding of vortex-antivortex pairs and the helicity modulus shows a finite universal jump. The origin of singular behavior in the small f limit is that a *depinned* Coulomb gas gives rise to metallic screening of the 2D Coulomb vortex-anti-vortex interaction at long length-scales, which means that thermally excited free vortices appear at any finite temperature, and the vortex unbinding transition is absent.

It would be interesting to know the critical value of the commensurate frustration, such that for all $f < f_c$, T_p lies below T_m. However it appears unlikely to us that $T_m = T_p$ for any $f < 1/56$ because $f = 1/56$ is particularly strongly pinned, since it has near hexagonal symmetry. It is also possible that depinning and melting transitions separate for some values of $f > 1/30$. While from our simulations we cannot rule out the presence of an hexatic phase for $T > T_m$, this was not observed in the LCG.[12]

In conclusion, the lattice Coulomb gas and frustrated XY models show qualitatively very similar melting and depinning phase diagrams in low vortex density (weak commensurate frustration) limit. In complete agreement with the arguments of Moore,[10] we find that thermal fluctuations of the vortex lattice destroy long range phase coherence in the continuum limit of the frustrated XY model at any finite temperature. On the other hand, the model shows a genuine thermodynamic phase transition, which can be identified with the disappearance of algebraic long range order in the gauge invariant current pattern corresponding to the vortex lattice structure.

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