

Incommensurability in the frustrated two-dimensional XY model

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To examine the properties of the frustrated XY model at an incommensurate field we have examined a sequence of magnetic filling factors f which approach the irrational value of one minus the golden mean. At all f studied, the system undergoes a finite-temperature ordering transition involving the freezing out of Ising-like domain walls. As one approaches incommensurability, the low-temperature phase of the system changes from the staircase states found by Halsey [Phys. Rev. B **31**, 5728 (1984); J. Phys. C **18**, 2437 (1985)] to a striped phase consisting of a superlattice of parallel shift (Pott's-like) domain walls. Our results suggest that the glassy effects previously reported for this model are an artifact of the boundary conditions and dynamics that were used. [S0163-1829(99)03426-8]

I. INTRODUCTION

The irrationality of a parameter f , characterizing the frustration of a physical system, can have a profound and often very surprising effect. In the frustrated XY model, the interplay of two length scales—the mean separation of vortices induced by the frustration f and the period of the underlying lattice—gives rise to a wide variety of interesting physical phenomena.¹ Halsey has proposed,² based on numerical evidence, that in the limit of an irrational $f^* = (3 - \sqrt{5})/2$ this model displays a glass transition to a superconducting frozen disordered vortex state. If this were true, it would make the frustrated XY model at f^* a structural glass, a glassy system which possess no intrinsic random disorder, something of great current interest. Experiments on superconducting arrays,³ an experimental realization of this model, find evidence for a finite-temperature transition for this irrational f^* . However, recent simulations by Granato⁴ showed results consistent with a glass transition at zero temperature, and those by Kim and Lee⁵ showed dynamics resembling that of a supercooled liquid near the transition temperature found by Halsey. In contrast, Gupta, Teitel, and Gingras²⁰ have recently studied the irrational Josephson array using the Coulomb gas formalism and find a first-order transition to an ordered state. In light of these conflicting results, it is important to clearly investigate which of these results holds for the frustrated XY model, originally studied by Halsey.

Naively, one might have expected this system to behave in a similar manner to the commensurate-incommensurate (C-I) behavior seen in the discrete sine-Gordon model.⁶ While this is the case for the frustrated XY model in a one-dimensional ladder geometry,⁷ global screening currents are required in order to maintain a vortex density different from the frustration f . Since in 2D this costs an energy logarithmic in the size of the system, fixed density of vortices equal to f is always observed, destroying the devil's staircase structure of the phase diagram (in the density- f plane). Since previous studies of C-I transitions have been done under conditions of fixed chemical potential (varying density) rather than fixed

density, it is unknown what effect this additional global constraint will have.

To study the system near incommensurability we examine a sequence of states, $f = 3/8, 5/13, 8/21, 13/34, 21/55, 34/89, \dots$, which approaches the quadratic irrational value of $f^* = (3 - \sqrt{5})/2$. We examine ground-state properties and low-energy excitations using a numerical constrained optimization to minimize the energy. We correlate these states to those found with Monte Carlo (MC) simulations of systems with *soft* boundary conditions. When we relax the constraint of fixed periodicity, allowing the system to find its own natural period, we find that the system undergoes a *finite temperature* (not approaching zero) phase transition to an *ordered* state. As one goes down this sequence towards f^* we find that at $f = 5/13$ the ground state changes from a staircase state^{8,9} to a striped phase, similar to those found in commensurate-incommensurate transitions. We therefore conclude that the “glassy” behavior seen by previous workers is an artifact of energy barriers in their particular dynamics and boundary conditions.

II. THE MODEL AND DOMAIN WALLS

The Hamiltonian of the frustrated XY model is

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

where θ_j is the phase on site j of a square $L \times L$ lattice and $A_{ij} = (2\pi/\phi_0) \int_i^j \mathbf{A} \cdot d\mathbf{l}$ is the integral of the vector potential from site i to site j with ϕ_0 being the flux quantum. The directed sum of the A_{ij} around an elementary plaquette $\Sigma A_{ij} = 2\pi f$ where f , measured in the units of ϕ_0 , is the magnetic flux penetrating each plaquette due to the uniformly applied field.

It is, in general, quite hard to study a system near incommensurability. For numerical work this is due to the large system sizes required; for $f = p/q$ a system of *at least* $q \times q$, and possibly much larger,¹⁰ is required, and by definition q

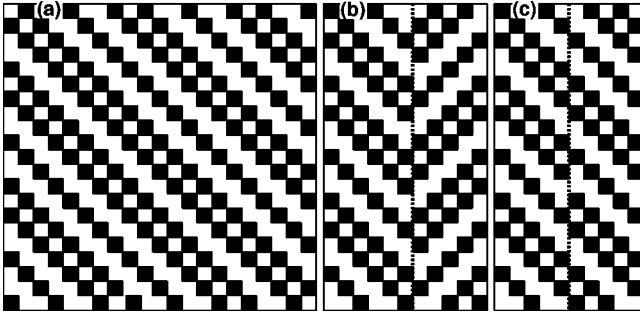


FIG. 1. Fluxoid pattern for $f = \frac{8}{21}$ for (a) a unit cell of the staircase state, (b) A herringbone wall, and (c) and shift-by-eight wall. A vortex is shown as a dark square. In (c), the pattern on the right is shifted down by eight from where it would be if it had just continued the pattern on the left.

$\rightarrow \infty$ for incommensurate f . The ground states of the Hamiltonian (1) will be among the solutions to the supercurrent conservation equations $\partial \mathcal{H} / \partial \theta_i = 0$:

$$\sum_{j'} \sin(\theta_{j'} - \theta_i - A_{ij'}) = 0, \quad (2)$$

where j' are the nearest neighbors to i . One set of solutions to these equations was found by Halsey⁸ in which the square network is partitioned into diagonal staircases with a constant current flowing along each staircase. The resulting fluxoid patterns consist of diagonal lines of vortices. A unit cell of the staircase fluxoid pattern for $f = 8/21$ is shown in Fig. 1(a). While these staircase states are not, as will be shown later, the ground states for all the f we study, they are still a useful set of states in that the striped phases we find near f^* can be defined in terms of domains of staircase states separated by parallel domain walls.

Figures 1(b) and 1(c) show some of the low-energy domain walls for a typical case, $f = 8/21$. Domain walls between the $2q$ degenerate staircase states can be classified into two types. *Shift* walls involve a shift of the vortex pattern across the wall [such as in Fig. 2(c) where the pattern on the right is shifted down by eight lattice spacings with respect to the pattern on the left] but the lines of vortices are still going along the same diagonal. *Herringbone* walls are walls between states with the vortex lines going along opposite diagonals. To calculate energies of different vortex patterns, we solved equations (2) numerically, using a quasi-

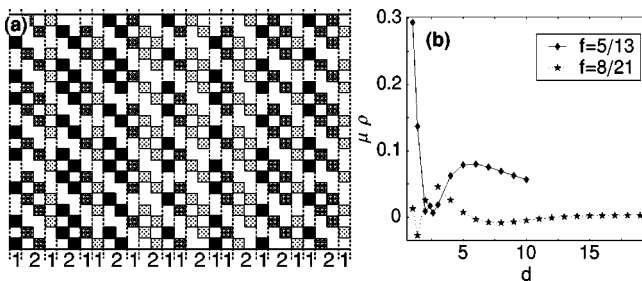


FIG. 2. (a) A section of the striped phase for $f = 8/21$ corresponding to the minimum in the energy in (b). The sequence of wall spacings repeats periodically. The shading is only a guide for the eye. (b) Energy per unit area of a superlattice of shift-by-eight walls as a function of their average separation for $f = \frac{5}{13}$ and $\frac{8}{21}$.

Newton method, on lattices with up to 2.3×10^5 sites and constraints fixing the fluxoid occupation of each plaquette. For $f = 3/8$ the lowest energy wall is a herringbone wall, but there is a shift wall with only slightly higher energy. For the higher-order rationals ($f = 5/13$ to $34/89$) there is at least one shift wall with lower energy than any single herringbone wall. In addition, a striped phase such as the one shown in Fig. 2(a), consisting of a superlattice of parallel shift walls is lower in energy than the plain staircase state for $f = 8/21$, $13/34$, $21/55$, and $34/89$.

The energy of a superlattice of parallel shift walls is shown in Fig. 2(b) for $f = 5/13$ and $8/21$. The presence of a short-range energetic repulsion makes wall crossings energetically unfavorable. Also, the interaction is essentially flat at large distances. There is, however, a minimum in the interaction potential at a finite separation of the walls which sets the period of the lowest energy state. This minimum arises due the directionality of the wall which causes the distortion of the phase to be asymmetric on each side of the wall. As a result, when the distortion of the phases from two walls overlap, there can be some cancellation. If however, the walls get too close, the distortions of the phase field from the two walls start to match, causing a rapid increase in energy.

III. BOUNDARY CONDITIONS

While energy calculations show that the striped phase is lower in energy than the plain staircase state for $f = 8/21$, $13/34$, $21/55$, and $34/89$, this does not necessarily mean that there is not some other state with even lower energy. To test this, we undertook extensive Monte Carlo simulations. Boundary effects can propagate quite far into the system as the boundary can easily induce a high-energy domain wall into the system if the period of the lattice does not coincide with the systems natural period. To alleviate this strain, the system will break this single high-energy interface into numerous lower energy walls resulting in a complicated structure of walls which can extend well into the system. These trapped domain structures will have a significant effect on finite-temperature states and transitions found in smaller samples. This problem is even more extreme when dominant excitations of the system cause the systems to have a period which depends on the presence or absence of the excitation. This is illustrated in Fig. 3. The ground state for $f = 3/8$ consists of the Halsey staircase state. However, close to the critical point a common excitation is a shift-by-three wall, as can be seen in Fig. 3(a). The state illustrated in Fig. 3(a) is very similar to the striped phases seen in more conventional commensurate-incommensurate (C-I) systems.⁶ However, one should notice that the number of shift-by-three walls is fixed to be a multiple of 8 if one imposes periodic boundary conditions, as we have done in this case. This is because each time one crosses a shift wall the vortex pattern shifts by three, and it requires eight shifts of three to bring the vortex pattern back in coincidence to what it would be without the walls. As one cools such a system further, the eight shift walls eventually condense into a superlattice of regularly spaced walls [Fig. 3(b)] with the spacing set by the minimum in the interwall potential [Fig. 3(c)]. This superlattice of shift walls then remains a very low temperature, even though it is

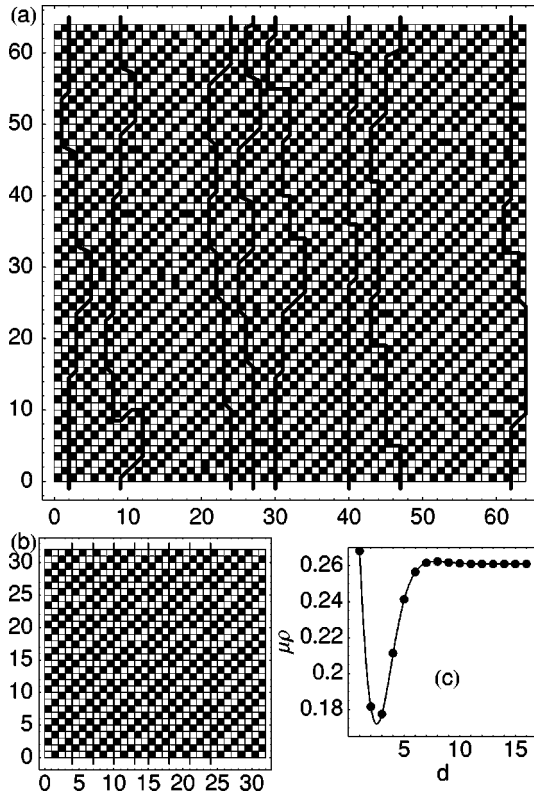


FIG. 3. (a) A vortex configuration produced from Monte Carlo simulation of $f=3/8$ with periodic boundary conditions and at $k_B T/J=0.122$. The system was started in the high temperature state and the temperature was lowered in steps of $\Delta T=0.003$ through the transition temperature, equilibrating at each step. (b) Similar to (a) except a smaller lattice and $k_B T/J=0.025$. (c) Energy per unit area of a superlattice of shift-by-three walls as a function of their average separation for $f=3/8$. Note that the spacing in (b) corresponds to the minimum energy.

clearly not the lowest energy state (the plain staircase state has lower energy). This is a result of the difficulty the system encounters in trying to rid itself of such configurations. In order to remove the shift walls, the system would have to do something like pinch all eight of them together to form a dislocation, as suggested by Schulz *et al.*¹¹ in the context of commensurate-incommensurate transitions. However, such an intermediate configuration appears to have an energy which is too high to be accessible without some global Monte Carlo moves (in other words, the core energy of such a dislocation is prohibitively high). Similar effects can be seen in other models such as the chiral clock model with the parameters so that domain walls do not wet each other.¹² A natural way for such directed walls to adjust their density is to enter or leave through the boundaries of the system. This would suggest some sort of free boundary conditions which do not fix the systems period. Free boundary conditions can however also induce domain walls, as a free boundary can act like a mirror plane in this system. To see this consider the $f=0$ case, which in the continuum limit has vortex excitations which are solutions to the Laplace's equation. The corresponding solution in a system with a free boundary has an image charge opposite the vortex across the boundary. As a result, even in the ground state a free boundary would induce a herringbone wall [cf. Fig. 1(b)] at the boundary.

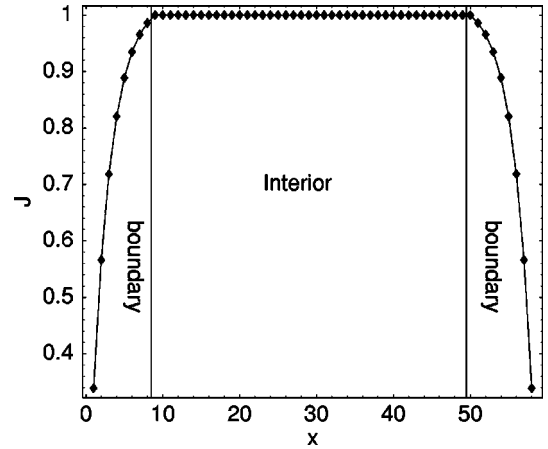


FIG. 4. Couplings J in a cross-section of the system for $L=42$. Data from the boundary layers is discarded.

In some sense, one can consider the boundary conditions to impose a hidden chemical potential which fixes the density of the shift walls. That the combination of frustration and this sort of global constraint could be the cause of the glassy behavior seen by other workers is not that surprising.

The problems of these boundary conditions can be alleviated by installing a boundary layer at the edge of the system. In the boundary layer, the coupling J in Eq. (1) goes from one on the interior side to zero on the exterior: $J(x)=A(1-e^{-x/\lambda})$ where $A=1/(1-e^{-w/\lambda})$ and w is the number of rows of lattice sites in the boundary layer and $\lambda < w$ is adjusted so that connection to the interior (where $J=1$) is reasonably smooth (see Fig. 4). We found that $w=8$ and $\lambda=2.5$ gave reasonable results. A similar type of approach was introduced by Olsson in Ref. 13, but we found that the more extended boundary layer we use here was more effective at allowing shift walls to move in and out of the boundaries. In practice, it would seem to be only necessary to use boundary layers in one direction and periodic boundary conditions can be kept in the other. This does lead to a preferred direction in the striped phase (stripes parallel to the boundary layers) and we shall mention the possible effects of this preference below. Measurements of the energy, order parameter, etc. were made only on the interior, where the coupling $J=1$.

IV. GROUND STATES AND PHASE TRANSITIONS

For the discrete degrees of freedom we kept track of an orientational order parameter M_d , measuring whether the vortices are preferentially arranged along one diagonal, and in the striped phase an order parameter ρ measuring the density of shift walls. The MC simulations used a heat bath algorithm with system sizes $32 \leq L \leq 96$. We computed about 10^7 MC steps (complete lattice updates), and data from different temperatures was combined and analyzed using histogram techniques.¹⁴

At the lowest temperatures of the simulations, $k_B T/J=0.03$, we find the system goes into the states expected from the energy calculations: $f=3/8$ and $5/13$ are in the plain staircase states and $f=8/21, 13/34$, and $21/55$ are in a striped phase. In the following discussion, we start by examining $f=8/21, 13/34$, and $21/55$ which undergo a phase transition at

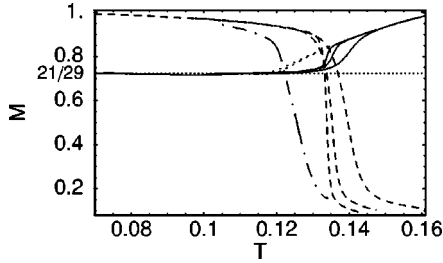


FIG. 5. Diagonal order (dashed) and shift wall density (solid) versus $k_B T/J$ for $f=8/21$ and $L=42, 63,$ and 84 for a system with periodic boundary conditions in one direction and soft boundary conditions in the other. Also shown is the diagonal order (dot-long dashed) for $L=84$ and shift wall density (dot-dashed) for $L=63$ and 84 versus $k_B T/J$ for $f=8/21$ for a system with soft boundary conditions in both directions. The fine dotted horizontal line indicates a shift wall density of $21/29$.

about $k_B T_c = 0.13J$ from the striped phase to the diagonally disordered phase. We then turn to the $f=5/13$ case which has a transition from the plain staircase state to the striped phase at $k_B T_c = 0.04J$ and then has a transition at $k_B T_c = 0.13J$ to a diagonally disordered phase. For the largest system sizes, $f=3/8$ appears to undergo a single transition from the plain staircase state to the diagonally disordered phase at about $k_B T_c = 0.123J$.

A. $f=8/21, 13/34,$ and $21/55$

Figure 5 shows the diagonal order and shift-wall density as a function of temperature for $f=8/21$. In the high-temperature phase, domain walls of all types, shift and herringbone, are present and the vortex lattice is disordered. At the critical temperature T_c , the system orders by freezing out herringbone walls, leaving a diagonally ordered striped phase. This striped phase has a density $\rho=21/29$ of shift walls almost independent of temperature (see Fig. 5). ($\rho=21/29$ corresponds to an average spacing of $1\frac{8}{21}$.) The non-integer spacing comes from a set s_{21} of two different wall spacings d_i of 1 and 2, arranged in a Fibonacci sequence cut off at 21; $s_1 = \{d_0\} = \{1\}$, $s_2 = \{d_0, d_1\} = \{2, 1\}$ and s_n is derived from the sets s_{n-2} and s_{n-1} as $s_n = s_{n-2} : s_{n-1}$, where the $:$ symbol indicates concatenation. So, for instance $s_3 = \{d_1, d_2, d_3\} = \{1\} : \{2, 1\} = \{1, 2, 1\}$. The full sequence to s_{21} is given along the bottom of Fig. 2(a). Note that it is the wall spacings that repeat periodically every 21 walls, but the actual vortex lattice period repeats every $29 \times 21 = 609$ lattice constants (one period of the wall spacings takes 29 lattice constants for $\rho=21/29$). Thus, the typical period of the ground-state vortex lattice becomes of order q^2 rather than q (recall $f=p/q$). The spacing observed in the Monte Carlo simulations corresponds to the system sitting at the minimum of the energy in Fig. 2(b). We should note that this is quite different from the case studied in commensurate-incommensurate transitions⁶ where there is no minimum in the interaction potential to pin the walls.

We now consider the order of the transition from the striped phase to the diagonally disordered phase as a function of temperature. One can see from Fig. 5 that there appears to be some difference between the behavior depending on the boundary conditions. This is very noticeable for the shift-

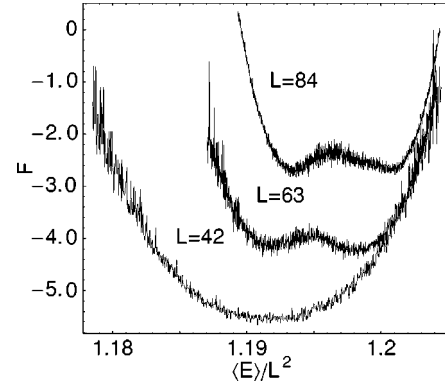


FIG. 6. Free energy versus energy, showing the free energy barrier between ordered and disordered state for $f=8/21$ and with periodic boundary conditions in one direction and soft boundary conditions in the other.

wall density, which has a bit of a jump when the boundary conditions are periodic in one direction and soft in the other (mixed) whereas the shift-wall density goes smoothly to $\rho=21/29$ when soft boundary conditions are applied in both directions. The order of the transition is most clearly indicated by examining the free energy at the transition, a technique described in Ref. 15. The free energy as a function of energy is obtained using $\mathcal{F}_L(E) = -\ln P_L(E)$ where $P_L(E)$ is the probability distribution for the energy E , generated by Monte Carlo simulation of a $L \times L$ system. Figure 6 shows that for mixed boundary conditions near the transition temperature, the free energy has two distinct minima, corresponding to the ordered and disordered states. The free-energy barrier between these two states grows as the system size increases from $L=42$ to 84 implying a first-order transition.¹⁵ However, this barrier does not appear to be present when soft boundary conditions are applied in both directions. Unfortunately, in neither case are the system sizes large enough to start applying finite-size scaling to confirm the nature of the transition. It may appear strange that the boundary conditions can effect the order of the phase transition. However, imposing a periodic boundary condition in one direction fixes the direction of the stripes. This might act like a (Z^2) symmetry-breaking field and might cause the transition first order. It is not clear if the barrier observed in Fig. 6 will continue to grow indefinitely. It is growing rather slowly compared to, say the barrier growth observed in the first-order phase transition seen for $f=2/5$,¹⁶ and it is possible it may reach a finite size and level off, so that the transition would also appear second order in the thermodynamic limit even for the mixed boundary conditions. In any case, substantially more work on larger systems is needed to resolve the situation. On the experimental side, the situation concerning the order of the transition is also ambiguous. Experimentally,³ a finite-temperature second-order phase transition is seen at $f=f^*$. That the transition occurs at finite temperature is in agreement with our results. But the observed continuous transition could be due to the presence of bond disorder which has been shown to wipe out any coexistence region of two phases in two dimensions making all transitions continuous.^{18,19}

The $f=13/34$ and $21/55$ cases also undergo a phase transition at around the same $T_c=0.13$ from the diagonally dis-

ordered high-temperature phase to the striped phase. The striped phases for these f appears to be slightly more complicated. Like the $f=8/21$ case, the stripes appear to be mainly composed of shift-by-eight walls with a similar Fibonacci sequence of spacings (with spacings of 2 and 3). However, these higher-order rationals also have other walls which have negative energy with respect to the staircase state. These additional walls also seem to be present in a much lower density, interspaced between the shift-by-eight walls in some quasiperiodic pattern. If one includes these walls, the wall density is similar to $f=8/21$ and the vortex lattices look very similar to $f=8/21$, which is probably why they have such similar T_c .

B. $f=5/13$

For $f=5/13$ the shift walls are the lowest energy walls, but the striped phase costs energy [see Fig. 2(b)]. The striped phase can exist at finite temperature however, due to entropic reasons which we shall discuss below. In the Monte Carlo simulations we see a very similar transition for $f=5/13$ (similar T_c) to the one seen for $f=8/21$ from the diagonally disordered high-temperature phase to the striped phase. The wall density in the striped phase is fixed at about $\rho=13/31$, which can be constructed from a Fibonacci sequence of wall spacings consisting of spacings of 2 and 3 in a manner similar to that used for spacings of 1 and 2 for $f=8/21$. For $L=39$, and at about $T\approx 0.05$ the wall spacings of 2 and 3 appear to switch to give a slightly lower energy state at $\rho=13/34$. It is unclear however if this would be the case for larger systems and would require further study. These two wall densities, $\rho=13/34$ and $13/31$ correspond to the two dips within the larger minima seen in the interaction energy shown in Fig. 2(b). At a lower temperature $T_p\approx 0.045$, the system undergoes a first order transition from the striped phase to the plain staircase state.

The transition from the plain staircase state to the striped phase is similar to the commensurate-incommensurate transitions studied in the context of adsorbed films,⁶ which is a second-order phase transition. In studies of these transitions, one considers the free energy of a single line per unit length ϵ_s . This can be estimated using a simple solid-on-solid (SOS) model of the shift line. The energy of the line, extending from one side of the system to the other is

$$\mathcal{H}_s\{z\} = \sigma_{\parallel}L + \sigma_{\perp} \sum_k |z_k - z_{k-1}|, \quad (3)$$

where σ_{\parallel} (σ_{\perp}) is the energy per unit length in the direction parallel (perpendicular) to the wall. The heights z_k , take on integer values. The partition function, can be evaluated to give the interfacial free energy per column¹⁷ $\epsilon_s = T \ln[e^{\sigma_{\parallel}/T} \tanh(\sigma_{\perp}/(2T))]$. A phase transition occurs when ϵ_s becomes negative. If this were the case here, one would see a continuous rise in the shift-wall density. What makes this case different is the presence of the minimum in the wall interaction potential [Fig. 2(b)] which we take into account in the following.

If placed in a system with other shift walls, the walls will experience an entropic repulsion since a wall can only occupy the region of space between its neighbors. To see

whether or not this entropic repulsion is relevant, we estimate if two walls remain bound together at the minima of the interaction potential. This is done using a SOS model for two walls with a binding energy equal to the depth of the minima in the interaction:

$$\mathcal{H}_d\{\Delta, z\} = \sum_k \{(2b\sigma + u_{\parallel} \delta_{z_k,0}) + b\sigma |z_k - z_{k-1}| + (2b\sigma + u_{\perp} \delta_{z_k,0}) \Delta_k\}. \quad (4)$$

where z_k is the separation of the walls ($z_k \geq 0$), and Δ_k is the number of vertical steps the two walls take in the same direction in the k th column ($-\infty < \Delta_k < \infty$). u_{\parallel} and u_{\perp} are the binding energies parallel and perpendicular to the wall. Summing over Δ_k leaves the partition function in the form of a transfer matrix: $\mathcal{Z} = \sum_{\{z_k\}} \prod_k T_{z_k}^{z_{k-1}}$. A ground-state eigenvector $\psi_{\mu}(z) = e^{-\mu z}$, where $1/\mu$ is the localization length, or typical distance separating the lines, characterizes the bound state of the two lines. $\mu=0$ defines the unbinding transition at T_b . Doing this, one finds an unbinding temperature of $k_B T_b / J = 0.51$. Below T_b , the entropic repulsion is insufficient to push the system out of the minimum. Above T_b , the striped ‘‘solid’’ phase will melt into a phase where the wall density changes continuously with temperature. Here, however, this is preempted by the entrance of the diagonally disordered phase at $T_c = 0.13J$.

In order for the striped phase to be stable for $f=5/13$, where it costs energy, there must be sufficient entropy from the lines wandering within the region between its neighbors. The energy per line at finite temperature can be estimated using Eq. (3) with z_k restricted to $0, \pm 1$ as the minimum in the interaction energy is at a spacing of about 2. The free energy per line per column is then

$$\epsilon_b = T \ln\{e^{\sigma_{\parallel}/T} / [1 + e^{-2\sigma_{\perp}/T} (1 + \sqrt{1 + 8e^{2\sigma_{\perp}/T}}) / 2]\}.$$

At the point where ϵ_b crosses zero the striped phase coexists with the plain staircase state and a first-order phase transition occurs. Taking $\sigma_{\parallel} = 0.041J$ for the shift-by-eight wall at the minimum of the interaction energy and $\sigma_{\perp} = 0.04J$ from an average of measurements of the energy of several kinks of differing lengths, one finds that ϵ_b crosses zero at $T_b = 0.04J$ in reasonable agreement with the value observed in the Monte Carlo simulations.

V. CONCLUSION

In conclusion, we find that all of the systems studied undergo a finite-temperature transition from an ordered state to a diagonally disordered state.²⁰ The transition temperature is nearly constant and shows no signs of approaching zero as one goes to more incommensurate f . As one approaches incommensurate f , the low-temperature state changes from the plain staircase state found by Halsey to the striped phase. We find that the choice of boundary conditions, at least in the finite-size systems available to study numerically, can have a significant impact on the dynamics. It does this by creating barriers for parallel shift walls, a dominant excitation in the low-temperature state. If one takes periodic boundary conditions near $f=f^*$ typically glassy behavior has been observed in simulations. If one takes the soft boundary condition that

allows the system to adjust the density of shift walls in one direction and the periodic boundary condition in the other direction, one obtains an ordered low-temperature state and what appears to be a weak first-order transition. If one takes

the soft boundary condition in both directions it would appear that one finds a continuous transition to the ordered low-temperature state. This final observation, one could argue, should be the true result in the thermodynamic limit.

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