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Ground state of the uniformly frustrated two-dimensional XY model near $f=1/2$

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Teitel and Jayaprakash have conjectured that the ground states for the uniformly frustrated XY model (a model for the Josephson network in a magnetic field) are periodic on a $q\times q$ cell when the frustration factor f (the magnetic flux measured in units of the flux quantum) is a rational number p/q. We have found examples for f close to 1/2 where a larger cell—apparently $2q\times 2q$—is required. We conjecture that something similar occurs whenever f is sufficiently close to a simple ratio.

I. THE UNIFORMLY FRUSTRATED MODEL

The uniformly frustrated two-dimensional XY model on the square lattice is described by the Hamiltonian

$$H=-J\sum_{i,j}\cos(\phi_{i,j+1}-\phi_{i,j})-J\sum_{i,j}\cos(\phi_{i+1,j}-\phi_{i,j}-\chi_j)\ , \tag{1}$$

where $\chi_j=2\pi fj \pmod{2\pi}$ is the frustration function. This is a model for an array of superconducting grains in a magnetic field; then H describes the Josephson coupling between the phases $\phi_{i,j}$ of the grains and χ_j represents the vector potential in the Landau gauge, with $f=a^2B/\Phi_0$ being the magnetic flux per unit cell of the lattice, measured in terms of the flux quantum Φ_0.

The ground states of Eq. (1) have been discussed by a number of authors.[1–4] When f is rational, described by integers p and q such that $f=p/q$, the frustration factor χ_j is periodic on the lattice with interval q; correspondingly Teitel and Jayaprakash[1] have conjectured that the ground-state phase distribution is periodic on a $q\times q$ square. This conjecture gives reasonable results for small q, and it is difficult to study the more exotic cases that arise when q is large; however, we believe that the underlying physics suggests some counterexamples.

Visualizing and understanding the spatial dependence of $\phi_{i,j}$ is hampered by the need to factor in the spatial dependence of χ_j, as well as the invariance under the transformation $\phi_{i,j}\rightarrow\phi_{i,j}+C$. It is preferable to study the pattern of the Josephson currents defined by

$$\begin{aligned} I_{ij}^x&=J\sin(\phi_{i,j}-\phi_{i+1,j}-\chi_j)\ ,\\ I_{ij}^y&=J\sin(\phi_{i,j}-\phi_{i,j+1})\ . \end{aligned} \tag{2}$$

In the ground state [and other local minima of Eq. (1)], these currents are conserved at every site. The current circulating around a unit cell of the lattice is small for most sites, but for a fraction f of the sites, the directed sum around the plaquette,

$$S=I_{i,j}^x+I_{i+1,j}^y-I_{i,j+1}^x-I_{i,j}^y\ , \tag{3}$$

is large (i.e., greater than unity); these plaquettes have resident vortices. For example, the ground state for $f=\frac{1}{2}$ has vortices on half of the plaquettes, arranged in a checkerboard pattern. Many of the ground-state configurations can be understood in a simple model which regards the vortices as being mutually repelling particles.

Halsey[3] has described a family of configurations for which

$$U=-(2J/q)\csc(\pi/2q)\ , \tag{4}$$

and conjectured that this is the ground-state energy for $f>\frac{1}{2}$. Teitel[4] has disproved this with a counterexample for $f=\frac{5}{11}$; however, this is still a useful result since it represents a rigorous upper bound.

II. GROUND STATES FOR F NEAR $\frac{1}{2}$

A specific example where the ground state is not periodic on $q\times q$ is the case $f=\frac{5}{11}$. This case is of interest because it is close to the maximally frustrated case $f=\frac{1}{2}$. Teitel[4] has found the minimum-energy configuration periodic on an 11×11 square; it consists of domains of checkerboard pattern of opposite registry with two vacancies. Its energy is quoted as $-1.294\,66$ per site (we have reproduced Teitel's state and find $-1.294\,758$, using double-precision arithmetic). Halsey's Eq. (4) would give $-1.277\,58$.

Our conjectured ground state is constructed from the uniform checkerboard pattern with a low density of vacancies (the density of defects is $f'=\frac{1}{2}-\frac{5}{11}=\frac{1}{22}$). This state violates the Teitel-Jayaprakash conjecture because the checkerboard pattern will not fit in a cell of odd edge, suggesting that the domain structure found by Teitel is an artifact of forcing the incommensurate boundary condition on the checkerboard pattern; thus we were led to study the 22×22 cell.

For any one variable $\phi_{i,j}$, it is easy to find the value that minimizes Eq. (1) with all other variables held fixed; iterating this over all sites many times quickly leads to a configuration which is stable against small perturbations, but generally is not the global minimum. Monte Carlo annealing, which shakes the system out of local minima by the introduction of a controlled amount of randomness, was tried; however, this is not an efficient way to perfect the configuration. It was useful in suggesting the optimum arrangement of vortices; we then found that we could "edit" the arrangement of phases by replacing the phases of the sites in a chosen 5×5 cell by the phases from another cell (adjusting these by a constant so that the phase at one corner was unchanged) and then relaxing the result to local equilibrium. In this way it was possible to eliminate the regions of incorrect registry and move the vacancies about, eventually attaining the state represented by Fig. 1, which has an energy of $-1.295\,650$ per site, slightly lower than Teitel's state.

This editing procedure does not necessarily produce a state with zero current—it may construct (or attempt to construct) a configuration with a persistent current circulating through the periodic boundary. Indeed, shifting a vortex pattern by one lattice spacing is equivalent to the introduction of a phase difference $2\pi fL$ across the system and gives rise to a current of the same order of magnitude. It should also be noted that any configuration that lacks inversion symmetry will have nonzero average current. Since current-carrying states have higher energy, Monte Carlo methods will tend to avoid these configurations. However, both in the editing approach and in Monte Carlo annealing, it is possible to have a "seed crystal" present, which will lead to a current-carrying state if completed by purely local changes in the phases. Thus, in constructing ground states by any method, it may be useful to check for the circulating current and correct for this condition when it arises.

The significance of this new ground state goes beyond

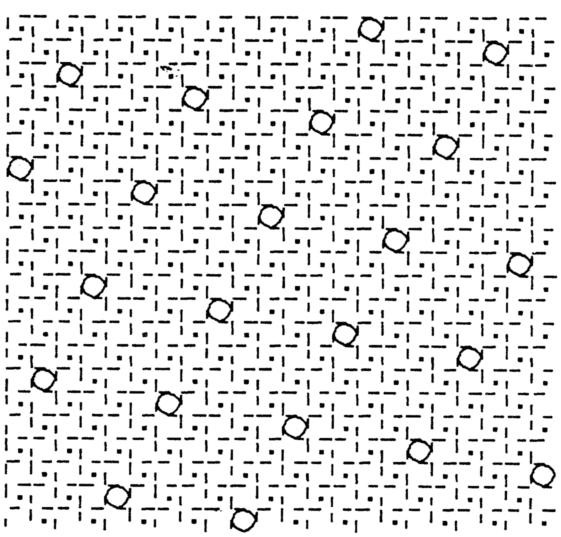

FIG. 1. Ground state for $f=\frac{5}{11}$. The short lines point along the bonds of the lattice and indicate the direction and magnitude of the current; the dots mark the plaquettes having vortices, and the circles are plaquettes which do not have vortices, but would in the $f=\frac{1}{2}$ checkerboard pattern.

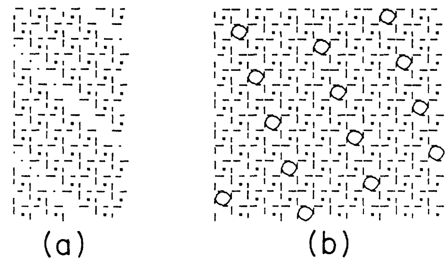

FIG. 2. Case $f=\frac{3}{7}$: (a) the ground state, periodic on 7×7; (b) a defect superlattice state periodic on 14×14.

the slight decrease in energy, because it has (in common with the states for smaller q and p) a periodic vortex structure, and thus the resistive transition can be understood in terms of the melting of the vortex lattice (or, in this case, the defect superlattice). The theory of the critical current is also different in the two cases: the mechanism which limits the phase strain that can be applied to the defected lattice is the motion of a vortex into a defect, which must go through a higher-energy state involving adjacent vortices and thus has a high critical current; a domain wall is easier to displace because it only entails recruiting vortices from one domain to the other.

We have verified these assertions by imposing a phase difference at the periodic join (as previously described[5]) and find that, for currents along one axis, the vortex lattice shown in Fig. 1 is stable up to a current density 0.184/bond, at which point some of the defects relocate (as the phase difference continues to increase, further relocation takes place, eventually regenerating the configuration of Fig. 1 displaced two lattice sites); a cor-

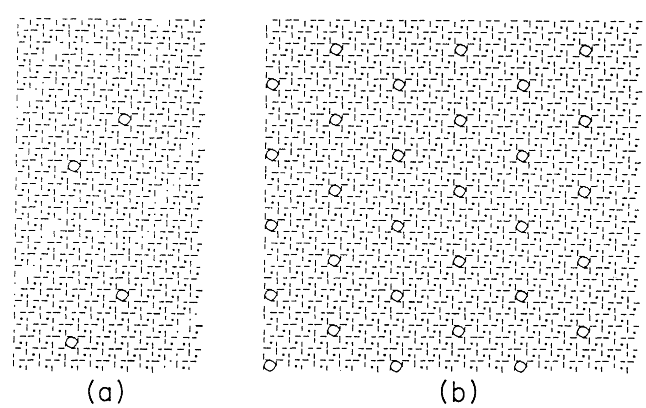

FIG. 3. Case $f=\frac{7}{15}$: (a) the lowest-energy state having 15×15 periodicity; (b) the ground state, with 30×30 periodicity.

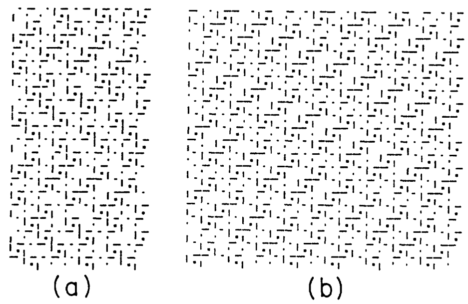

FIG. 4. Case $\frac{3}{10}$: (a) the lowest-energy state having 10×10 periodicity; (b) the ground state, with 20×20 periodicity.

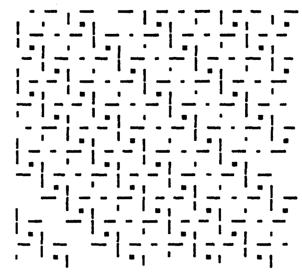

FIG. 5. Ground state for $\frac{4}{11}$.

responding study of the Teitel state found a critical current 0.115, with the initial motions being displacements of the domain wall.

We have sought to generalize this construction to other f. The most likely and obvious cases are for f close to $\frac{1}{2}$. We have succeeded in constructing the analogous configuration for $f=\frac{3}{7}$, but its energy density (-1.2601) is greater than the ground state ($E/N=-1.2840$) found by Teitel and Jayaprakash (Fig. 2). (Halsey's expression also gives this value.) For $\frac{7}{15}$ the best configuration that we have found on 15×15 has an energy density of $-1.312\,18$ (Fig. 3); we find a structure on the 30×30 square with an energy density of $-1.316\,444$ (this case was chosen with the anticipation that this nearly hexagonal structure would have a low energy). These three examples help characterize how close to $\frac{1}{2}$ f must be: The defect superlattices have a length scale of at least several lattice spacings.

It was also noted for $f=\frac{7}{15}$ on 30×30 that the energy difference between the ground state and the state with one defect displaced one plaquette diagonally (that is, to the nearest available position) is higher by 0.428, whereas the corresponding defect in the $f=\frac{1}{30}$ arrangement (which has vortices at the positions that $f=\frac{7}{15}$ has vacancies in the vortex checkerboard pattern) has $\Delta E=0.576$. This suggests that vortex-lattice melting temperatures (i.e., the resistive transitions) are comparable.

These examples, together with previously published ground-state configurations, support the observation that the current pattern and vortex structure have a unit cell which is much smaller than $q\times q$ (typically its *area* is q) and from this point of view our observation is that close to $f=\frac{1}{2}$ its area should also be even for consistency with the $f=\frac{1}{2}$ structure.

When using periodic boundary conditions, it will always be necessary to use panels whose width is a multiple of q, because this is the period of χ_j; however, this is of doubtful relevance to the periodicity of gauge-invariant quantities such as the currents. In any case the periodicity rules seem to be more closely related to the minimum-energy configurations of a gas of particles interacting with a potential which is repulsive and somewhat anisotropic at short distances (where it is weaker in the diagonal direction). Thus the unit cell for Fig. 3(b) is a centered rectangle having edges 10 and 6, neither of which divide 15.

The energy densities for the three examples of vacancy superlattices found here can be fitted with the expression

$$U=-1.414-(\tfrac{1}{2}-f)[-0.501-\ln(\tfrac{1}{2}-f)]\ , \qquad (5)$$

in which the first term is the energy density at $f=\frac{1}{2}$ and the correction describes a distribution of vacancies with a logarithmic repulsive potential. Comparison of this expression with Halsey's (which is essentially constant for $q>10$) shows that the vacancy superlattice has lower energy for $f>0.45$.

III. OTHER VALUES OF Q

The $f=\frac{1}{2}$ checkerboard pattern is special because its excitations (i.e., defects and reverse-registry domains) are relatively high energy. In contrast, the ground states for other f have low-energy excitations (for example, the ground state for $f=\frac{1}{3}$ consists of diagonal chains of vortices, and there are configurations with kinked chains that have only slightly higher energy), and their more complex structures allow other ways to incorporate the defect structure. For example, we have studied the case $f=\frac{3}{10}$, which is slightly less than $f=\frac{1}{3}$, in hope of demonstrating a 30×30 periodicity with nine vacancies in a $f=\frac{1}{3}$ structure. The best structure we have found that is periodic on 10×10 has no smaller periodicity; its energy density is $-1.320\,12$. On 30×30 we were unable to force the construction of the proposed configuration and could only find configurations with slightly lower energy density ($-1.320\,25$). However, on 20×20 we found the structure shown in Fig. 4, with an energy density of -1.3275. The current pattern is periodic on 10×10, but the phases are not, so that $\phi_{i,j}=\phi_{i,j+10}+\pi \pmod{2\pi}$. This rather surprising example represents a second mechanism for periodic doubling. It also points out that for smaller f there are more ways to alter the local density of vortices. For $f=\frac{4}{11}$ we have found a structure that interpolates between $f=\frac{1}{3}$ and $\frac{1}{4}$ (Fig. 5) and is periodic on 11×11. There is still the possibility that, for f closer to $\frac{1}{3}$ (e.g., $\frac{333}{1000}$), the $f=\frac{1}{3}$ structure with a vacancy superlattice will eventually appear.

ACKNOWLEDGMENTS

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