UNIFORMLY FRUSTRATED xy MODELS: GROUND STATE CONFIGURATIONS

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The ground state vortex configuration of the uniformly frustrated xy model in two dimensions is studied with Monte Carlo simulations. A considerably more complicated structure is reported than found previously.

In this paper we present numerical results for the ground state vortex configuration for the uniformly frustrated two-dimensional xy model [1, 2]. Our results indicate that the ground state is considerably more complicated than has been suggested previously [3].

We have introduced the uniformly frustrated xy model to describe behavior in two-dimensional Josephson junction arrays [1, 2]. The Hamiltonian is given by:

$$H = J \sum_{\langle ij \rangle} \cos(\sigma_i - \sigma_j - \chi_{ij}) , \qquad (1)$$

where σ_i is the phase at node *i*, and χ_{ij} is a gauge variable related to the integral of the vector potential across junction $\langle ij \rangle$:

$$\chi_{ij} = \frac{2e}{\hbar c} \int_{i}^{l} A \cdot \mathrm{d}l \,.$$

The key parameter of the theory was shown to be the uniform frustration f, where

$$2\pi f = \chi_{ij} + \chi_{jk} + \chi_{kl} + \chi_{ll}$$
 (2)

is the sum of gauge variables about any unit cell of the lattice. In terms of a uniform applied transverse magnetic field H_0 , $f = H_0 a^2 / \Phi_0$, the number of flux quanta per unit cell.

The gauge field χ introduces vortices in the phase variables σ_i , with average vortex density f. In the ground state, these logarithmically repelling vortices organize into an ordered structure. For the $f = \frac{1}{2}$ ground state, a vortex sits in every other cell of the lattice and so the ground state is

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doubly degenerate [1]. In a previous paper [2] we presented ground state configurations for several values of f. If f = p/q, p and q coprime integers, then for q small and $\frac{1}{3} < f < \frac{1}{2}$ the ground state was seen to have a particularly simple form. The ground state could be described by striped domains of the two $f = \frac{1}{2}$ ground states separated by straight domain walls running diagonally through the system. In a recent paper [3], Halsey, by assuming such a straight domain wall structure for general $\frac{1}{3} \le f \le \frac{1}{2}$, calculates the ground state energy E and finds for f = p/q;

$$E(p/q) = -J \cdot \frac{2}{9} \operatorname{cosec}(\pi/2q), \qquad (3)$$

i.e. E depends only on q and thus is a highly discontinuous function of f. Our Monte Carlo results and physical arguments, presented below, demonstrate this assumption to be incorrect.

In fig. 1 we present results from Monte Carlo simulations for the ground state vortex configuration at $f = \frac{5}{11}$. The unit cell of the ground state is 11×11 and for clarity we show a 2×2 cell structure. Solid dots represent a vortex, heavy lines represent a domain wall between the two $f = \frac{1}{2}$ ground state structures, and an open circle represents a vacancy in the $f = \frac{1}{2}$ structure. As is seen, the domain walls are not straight, but wave in and out. While we cannot prove that Monte Carlo has given us the true ground state, we observe that the energy of the pictured configuration is E = -1.29466J which is lower than the straight wall configuration as computed from eq. (3): E = -1.27758 J. Thus, we feel the picture of waving domain walls in the ground state to be correct.

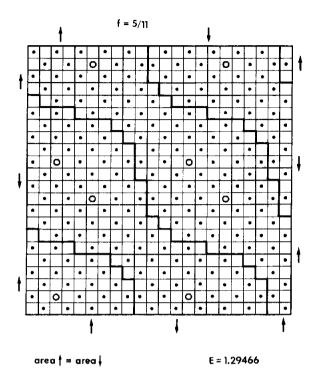


Fig. 1. Ground state vortex configuration for f = 5/11 from Monte Carlo simulations. The unit cell is 11×11 and a 2×2 cell structure is shown. Dots represent a vortex, heavy lines are domain walls between f = 1/2 like structures, and open circles are vacancies in a f = 1/2 like structure.

This result we find physically reasonable as well. Using the Coulomb gas analogy to vortices, we see that domain walls correspond to an excess charge density. For a vortex structure of density f to be approximated by domain of a simpler

structure f_0 (i.e. f = p/q, $f_0 = p_0/q_0$, $f \approx f_0$ and $q_0 \ll q$), the excess change density to be made up in defects is $f - f_0$. The model of Halsey puts this charge into straight parallel domain walls whose separation increases as $f \rightarrow f_0$. However, due to the long-range interactions between changes, the energy associated with two walls infinitely far apart remains finite and so $\lim_{f\rightarrow f_0} E(f) \neq E(f_0)$. This is the origin of the discontinuities in E(f) as computed by Halsey. The combination of wavy walls and vacancies as in fig. 1, however, spreads this charge more evenly and thus reduces the energy. (We may even speculate that for certain f, the wavy wall structure undergoes a transition to a checkered domain structure as walls cross.)

We therefore strongly believe that the straight domain wall model applies only to a very few simple f = p/q with small q. Most f will have a more complicated wavy wall structure, and we believe that once this is taken into account, the ground state energy will be a continuous function of f qualitatively similar to that given by the Gaussian approximation to (1) (ref. [4]) as calculated by Hofstadter [5].

References

- S. Teitel and C. Jayaprakash, Phys. Rev. B 27 (1983) 598.
- [2] S. Teitel and C. Jayaprakash, Phys. Rev. Lett. 51 (1983) 1999.
- [3] T.C. Halsey, Phys. Rev. B 31 (1985) 5728.
- [4] S. Teitel and C. Jayaprakash, J. de Physique Lett. 46 (1985) L-33.
- [5] D.R. Hofstadter, Phys. Rev. B 14 (1976) 2239.