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First- and Second-Order Phase Transitions in the $d=2$ XY Model

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The $d=2$ XY model is generalized to include an operator that couples directly to the vortex core energy, while maintaining the full symmetry of the original model. In addition to the usual Kosterlitz-Thouless transition, the model exhibits a true first-order transition and a *pseudo* first-order transition. The excitations of the model include fractionally charged vortices. Implications for the $d=2$ melting problem are discussed.

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In the controversy concerning the nature of melting in two dimensions,[1-7] the question at issue has generally been phrased in terms of whether or not the phase transitions are qualitatively the same as for the XY model.[1,2] The XY model can be approximately mapped onto the $d=2$ Coulomb gas and the transition is expected to be continuous, as described by the theory of Kosterlitz and Thouless (KT).[1] Since there is evidence from computer simulations that the melting transition is first order,[4,5] this analogy has been called into question.

However, it is possible to turn the question around and ask whether *all* transitions in XY models are actually described by the KT theory, or whether a first-order transition is also possible without disturbing the essential symmetry. To investigate this aspect of the problem, I have generalized the XY model by introducing an operator that couples directly to the core energy of the vortices (which map onto unit charges in a Coulomb gas). This is useful both because the assumptions of the KT theory might break down for small core energies[1,2,6,7] and in light of the interesting evidence presented recently by Saito,[7] suggesting that reducing the core energy in a dislocation vector system can change the transition from KT to first order.

For the generalized XY model, I have found true first-order transitions as well as KT transitions. This implies by analogy that two-dimensional melting could be either first order or continuous, depending on the parameters of the model, even if there is no fundamental difficulty with the analogy.

I have also found a *pseudo* first-order transition. This is really composed of (at least) two transitions, which cannot be resolved by standard computer-simulation techniques. By analogy, this implies that the nature of the melting transition in a given model probably cannot be decided by standard computer-simulation procedures.

Consider the Hamiltonian, $H=H_1+H_x$, for classical, two-dimensional spins of unit length, $\vec{\sigma}_i$, on a square lattice, where

$$H_1=K_1\sum_{<i,j>}\vec{\sigma}_i\cdot\vec{\sigma}_j \tag{1}$$

is the usual nearest-neighbor exchange and a factor of $-1/k_BT$ has been absorbed into the coupling constant. A "crossed-product" operator S_x is defined by

$$H_x=K_xS_x$$
$$=K_x\sum_{\text{plaquettes}}(1-\vec{\sigma}_i\cdot\vec{\sigma}_k)(1-\vec{\sigma}_j\cdot\vec{\sigma}_l), \tag{2}$$

where the corners of an elementary square (or plaquette) are labeled sequentially with i, j, k,

and l and each scalar product involves spins at opposite corners of a plaquette.[8] The operator does not affect the harmonic term in a expansion of the Hamiltonian for small fluctuations and only couples to spin waves in higher order.

For a simple, zero-temperature vortex or antivortex, the crossed-product operator has a contribution of $4.0K_x$ from the central plaquette, but only $0.3056K_x$ from each of the four nearest-neighbor plaquettes and a total of less than $0.16K_x$ from all more distant plaquettes. The full core-energy shift is $5.382K_x$.

For negative K_x, vortices are energetically less favorable. The effective fugacity is lowered, improving the validity of the KT assumptions.

For positive K_x, the model displays a variety of interesting phenomena. Perhaps the most startling effect is the appearance of fractionally charged vortices, with properties reminiscent of quarks. Starting from the vortex-antivortex pair shown in Fig. 1, a very short Monte Carlo (MC) run with $K_1 = 20.0$ and $K_x = 9.5$ produced the configuration shown in Fig. 2. The local minimum in the energy when the spins on opposite corners of a plaquette are antiparallel has produced vortices with charge one-half.[9] There are two energy contributions depending on the vortex-antivortex separation: a logarithmic term with effective charge one-half, and a linear term (confinement) due to the line of plaquettes with reversed spins. For very large separations, the linear term dominates and the system reverts to vortices with unit charge.

A related phenomenon is that isolated vortices change their shape when K_x is sufficiently large: The central vortex plaquette becomes a line of plaquettes with reversed spins to take advantage of the crossed-product operator. The resulting structures, shown in Fig. 3, look very much like domain boundaries and might not be recognized in a computer simulation as being vortices. Such large structures require a great deal of time to be created and annihilated.

For increasingly positive K_x, vortices become energetically more favorable and, for very large K_x, the model enters a new phase in which every plaquette contains a "vortex." For the melting problem, a high density of vortices would mean some sort of disordered phase. Because the XY model is confined to a lattice, the "vortex phase" has local antiferromagnetic order on each of the two square sublattices. In the ground state, the nearest-neighbor exchange cancels and the relative orientation of the two sublattices is arbitrary. For finite coupling constants, "ferromagnetic" fluctuations cause the spins to line up locally in rows.

Mean-field theory predicts a first-order transition between the vortex and ferromagnetic phases at $K_1 = 2K_x$ for large K_x. The behavior is probably not this simple and there may well be two second-order transitions. Leaving this question for a future publication, I simplify matters by adding an interaction between sites two lattice constants apart in the x or y directions (third-nearest neighbors) in analogy to Eq. (1). A true first-order transition is imposed by a positive value of K_2, stabilizing both the vortex and ferromagnetic

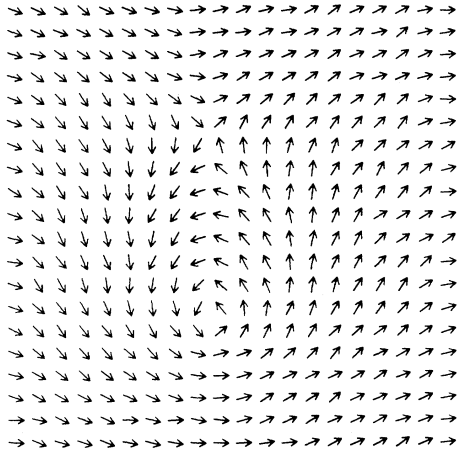

FIG. 1. 20× 20 spin configuration with a vortex-antivortex pair.

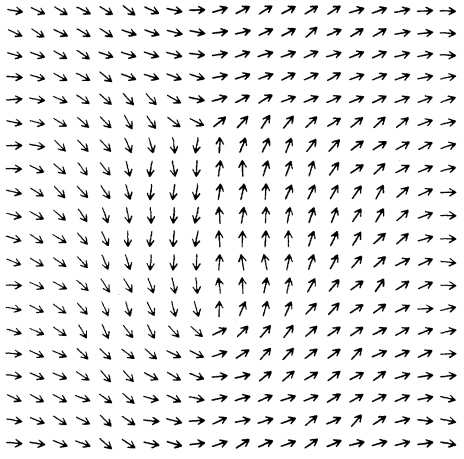

FIG. 2. Starting with Fig. 1, 40 MC steps/site at $K_1 = 20.0$ and $K_x = 9.5$ produced a vortex-antivortex pair with charge one-half. Tracing a path around a half-vortex, the spins rotate only 180 deg.

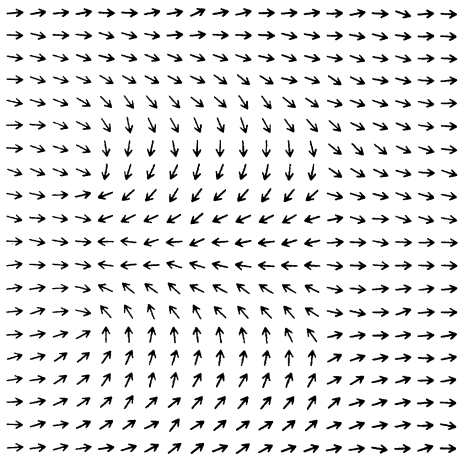

FIG. 3. The 20×20 spin system with a diagonally separated vortex-antivortex pair relaxed for 1500 MC steps/site with $K_1 = 20.0$ and $K_x = 9.5$. The vortex and antivortex have been "flattened."

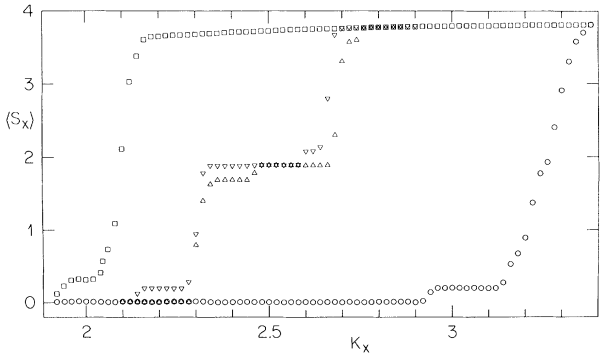

FIG. 4. Hysteresis for a 40×40 lattice with $K_1 = 5.0$ and $K_2 = -0.2$. Each point represents 500 MC steps/site. Increasing and decreasing K_x are represented by circles and squares for a MC simulation with single-spin processes only, and by triangles and inverted triangles for a modified algorithm, including reversal of one or two entire rows or columns. Differences for K_x between 2.1 and 2.5 are due to slowly diffusing pairs of domain walls. Extra runs without row reversals were made in the "wrong" phases at $K_x = 2.72$ and at $K_x = 2.26$. No sign of a transition to the stable phases was found for 10^4 MC steps/site.

phases with respect to the reversal of a line of spins.

A negative value of K_2 separates the ferromagnetic and vortex phases and inserts a phase for which the ground state has two rows of spins pointing in one direction alternating with two rows pointing in the opposite direction. Even within mean-field theory, there is no longer only a single transition.

However, a standard MC simulation of this system for $K_1 = 5.0$ and $K_2 = -0.2$ shows a single first-order transition as a function of K_x in Fig. 4. The hysteresis and the magnitude of the apparent jump are both large. The MC data in Fig. 4 would normally be taken as good evidence for a first-order transition, similar to that available for the problem of two-dimensional melting. Since there are really two transitions and an extra phase for the model considered here, standard computer simulations are not reliable for determining the order of a transition in such problems. The nature of the difficulty implies that even large increases in system size and simulation time would not remedy matters.

The presence of the intermediate phase can be demonstrated by constructing a generalized MC algorithm that also allows one or two entire rows or columns of spins to be reversed. MC data including this algorithm are also given in Fig. 4, and show transitions to the expected intermediate phase.

In summary, the variety of phase transitions in a generalized XY model suggests that the melting transition can be either first order or continuous, depending on the specific system. This is in agreement with the conclusions previously reached by Saito.[7] This picture is also in accord with the experiments of Heiney *et al.*,[10] in which they found that the melting transition for xenon on graphite can be either first order or continuous, depending on the xenon coverage.

Moreover, the relative simplicity of the XY model exposes an additional complication. Even when there really is an intermediate phase, the large spatial extent of the excitations and the long relaxation times can conceal the true behavior completely, giving the appearance of a single, first-order transition. This precludes the unambiguous determination of the nature of the transition in similar models with standard computer-simulation methods.

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Heavy-Neutrino Search Using $K_{\mu 2}$ Decay

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The muon momentum spectrum in $K_{\mu 2}$ decay has been measured by using a high-resolution magnetic spectrograph to look for a discrete muon peak associated with heavy-neutrino emission. The spectrum revealed no distinct peak, and the upper bound of the mixing ratio between the muon neutrino and a massive neutrino has been determined to be 10^{-4}–10^{-6} in the mass range of 70–300 MeV/c^2.

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Neutrinos are generally considered to be massless in the conventional theory of weak interactions. Experimentally, a finite neutrino mass cannot be excluded, especially if we take seriously the nonzero value of 14–46 eV/c^2 reported for the electron neutrino.[1] For other types of neutrinos, the present limits are $m(\nu_\mu) < 0.57$ MeV/c^2,[2] and $m(\nu_\tau) < 250$ MeV/c^2.[3]

Finite (and nondegenerate) neutrino masses imply neutrino flavor mixing since the weak neutrino eigenstates ν_e, ν_μ, and ν_τ are, in general, not mass eigenstates themselves, but linear combinations of the neutrino mass eigenstates as

$$\nu_l = \sum U_{li} \nu_i \quad (l = e, \mu, \tau, \ldots; \; i = 1, 2, 3, \ldots).$$

The current belief is that the mixing matrix is nearly diagonal, i.e., ν_e is dominantly coupled to ν_1, $\nu_\mu \cong \nu_2$, and $\nu_\tau \cong \nu_3$. In a series of papers Shrock[4] emphasized that there is a very interesting possibility that some of the neutrino mass eigenstates including unknown generations are so heavy that they may show up with probability $|U_{li}|^2$ in a two-body decay spectrum, well separated from the dominant peak. Such a possibility cannot be excluded by the presently known experimental evidences. On the other hand, neutrino-oscillation experiments[5] are only sensitive to small mass differences with relatively large mixing, and thus they cannot detect small mixing of heavy neutrinos.

A sensitive test of this interesting idea was proposed by Shrock, and involves measuring the lepton momentum spectrum in two-body leptonic decays of pseudoscalar mesons, such as K_{l2} or π_{l2}.

