Vortices and strings: Phase transition in anisotropic planar-rotor systems

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We have investigated the phase transition of a two-dimensional system described by the Hamiltonian $H=-J\sum_{\rm NN}\cos(\theta_i-\theta_j)-K\sum_{\rm NN}\cos(\theta_i+\theta_j+\phi_{ij})$, for $J,K>0$ and $0\le K/J\le 1$, and where NN denotes nearest neighbors, which has both Ising-like domain-wall (string) and XY-like vortex excitations. Migdal-Kadanoff and Monte Carlo renormalization-group studies indicate that there is only one transition which is Ising-like. The roles of string and vortex excitations in the phase transition are discussed by an energy-entropy argument and are found to be consistent with Monte Carlo quench results.

In recent years there has been considerable interest[1] in two-dimensional (2D) or quasi-2D physical systems consisting of molecules adsorbed on a surface. Under certain physical conditions,[2] the intermolecular interaction V_{ij} can be written in the form

$$V_{ij}=V_0-J_{ij}\cos(\theta_i-\theta_j)-K_{ij}\cos(\theta_i+\theta_j+\phi_{ij})$$
$$-A_{ij}[\cos(\theta_i+\phi_{ij})+\cos(\theta_j+\phi_{ij})]\ , \qquad (1)$$

where θ_i is related to the orientation of the ith molecular axis and ϕ_{ij} is an angle describing the orientation of the intermolecular bond with respect to a preferred anisotropy axis. The simplest Hamiltonian arising from V_{ij} is of the form

$$H=-J\sum_{NN}\cos(\theta_i-\theta_j)-K\sum_{\rm NN}\cos(\theta_i+\theta_j+\phi_{ij})\ . \qquad (2)$$

The above Hamiltonian reduces to the well-known isotropic planar-rotor (classical XY model) model for $K=0$. It was used to study the properties of N_2 molecules on a graphite substrate for particular values of J and K.[3] However, a detailed study of the properties of H in the entire parameter space is lacking and should be extremely interesting from a theoretical point of view because of the role of topological defects in the phase transition of 2D systems.

In this paper we discuss the nature of the phase transition for H given in Eq. (2). For simplicity we choose $J>0$, $K>0$, and $\epsilon=K/J<1$ and assume the rotors to be on a square lattice. A special feature of (2) for this case is that it allows for vortex excitations and yet has the simplest, namely two, domain pattern. In particular, we investigate (a) the effect of the interaction anisotropy ($K\neq 0$) on the Kosterlitz-Thouless (KT) transition, (b) the physical mechanisms underlying the order-disorder transition for 2D anisotropic rotors, and (c) the interplay of vortex and domain-wall excitations. The study of this interplay as a function of anisotropy is particularly important because of the role the domains play in the two phase transitions seen in XY model with *single-site* anisotropy of the form $H_p\cos(p\theta)$,[4] and isotropic p-state clock models (Z_p) for $p\ge p_c>4$. For the latter systems, Einhorn *et al.*[5] have argued that in the low-T ordered phase vortex-antivortex (V-A) pairs are bound to each other via strings (domain boundaries) which become floppy at a temperature T_1. This results in a loss of long-range order but the V-A pairs are bound to each other through a logarithmic potential leading to a KT-like phase which is then destroyed by the unbinding by V-A pairs at a higher temperature T_2. However, for the Z_p models, the two-domain system ($p=2$) does not have vortex excitations, and when the vortex does appear ($p\ge 4$), the domain-wall structure is quite complicated for simulation studies.[6] Therefore, Z_p models are not ideally suited for studying the interaction between domains and vortices.

The ground state of H is a doubly degenerate ferromagnetic state with $\langle\cos\theta_i\rangle=+1$ (or -1) for all i. At low T, the orientational correlation function $g(\mathbf{r})$ between the rotor at i and $i+r$ can be obtained by spin-wave approximation.[7] For $K=0$, $g(\mathbf{r})\to 0$ as $r\to\infty$ but for $K\neq 0$, $g(\mathbf{r})\to\eta^2$ as $r\to\infty$, where η is the long-range order (LRO) parameter. We find that $\eta\propto e^{-CT}$ for $K\simeq J$ and $\propto(K/J)^{DT}$ for $K\simeq 0$, where C and D are constants.

To get a general idea about the phase diagram for H we have used the Migdal-Kadanoff renormalization-group (MKRG)[8] procedure. We first move the vertical bonds and decimate the horizontal ones by integrating the partition function directly, and then move the bonds horizontally while decimating the vertical bonds. After these two operations, we take an average to restore the symmetry of the renormalized Hamiltonian H'. As a check of the reliability of the above procedure, we have applied it to the model with single-site anisotropy.[4] When $h_p=0$, there are two regions of J: in one the coupling iterates to zero directly, but in the other, it first increases to a certain value, then decreases very slowly to zero. For $p=6$, it appears that there are three regions: one in which J goes to zero but h_6 goes to a fixed value, in the second both J and h_p grow to infinity, and in the third (intermediate region) J first increases and then decreases slowly. This is consistent with the findings of Jose *et al.*[4]

For our model, we find that as long as $K\neq 0$ ($K/J=0.0001$), only after 10–20 iterations, the renormalized Hamiltonian H' can be represented by a simple form

TABLE I. Transition temperature $T_c^*=k_BT_c/J(1+\epsilon)$ using Migdal-Kadanoff and Monte Carlo renormalization-group analysis; critical exponents ν are for different values of the anisotropy parameter $\epsilon=K/J$.

ϵ	MKRG T_c^*	MCRG T_c^*	ν	ν_{Ising}	ν_{XY}
0.01	1.02	1.04	1.00±0.04	1.0	∞
0.10	1.18	1.20	0.97±0.09	1.0	∞
1.00	1.32	1.34	1.04±0.08	1.0	∞

$$H'=-J_x'\sum_{\langle NN\rangle}\cos\theta_i\cos\theta_j-A'\sum_i\cos2\theta_i\ , \tag{3}$$

with a small correction of the form $\sum_p A_p\cos(p\theta)$, $p>2$. There exists a temperature T_c, such that for $T<T_c$, both J/k_BT and A/k_BT iterate to infinity ($T=0$ fixed point); for $T>T_c$, A/k_BT iterates to a fixed value while J/k_BT approaches zero, suggesting that the system iterates to a noninteracting Ising spin system. The transition temperatures predicted by MKRG are in reasonable agreement with those given by Monte Carlo renormalization-group (MCRG) calculations (see Table I and discussion below).

To study the thermodynamic properties of H and to substantiate our MKRG results, we have performed Monte Carlo (MC) simulation of finite $N\times N$ systems with $N=16$ and 32. The number of MC steps/spin (MCS/s) were usually 5000–8000. Near the critical temperature 1.1×10^4 MCS/s were discarded and 1.2×10^4 MCS/s were used to compute thermal averages. Calculation of thermodynamic quantities such as average magnetization (η), specific heat (C), and susceptibility (χ) indicated that the system shows only one phase transition for three values of K/J chosen in our simulation (0.01, 0.1, 1.0). We have found that C and χ tend to peak at the same temperature, suggesting that the transition is Ising-like. In contrast, for $K=0$, it is believed[9] that C peaks at a temperature slightly higher than $T_c=T_{\text{KT}}$ where χ diverges.

Since it is difficult to locate the transition temperature from the T dependence of thermodynamic quantities in simulation studies in finite-size systems, we have used the MCRG procedure proposed by Skenker and Tobochnik[10] to find T_c. The essential feature of this procedure is the following: One starts from two systems of different size, say, 1024 spins and 256 spins; sums the spin around a plaquette vectorially; and then normalizes the sum to obtain the block spin. Next, thermodynamic quantities are calculated and matched for two block spin lattices of same size but originating from different systems. If T_1 is the temperature of the original larger system and T_2 of the smaller one, when the thermodynamic quantities of block spins match, then $\Delta T(=T_2-T_1)=0$ is a critical point, $\Delta T<0$ is an ordered phase, and $\Delta T>0$ is a disordered phase. The correlation-length critical exponent ν can be derived from this information.[9]

In Fig. 1 we plot the nearest neighbor correlation functions for 8×8 block spin lattices obtained from the two systems, the larger one (32×32) denoted by ○ and the smaller (16×16) denoted by ●. The crossing of the two curves gives the transition temperature T_c and it only shows one phase transition. In Table I, we give the value of T_c measured in units of $J(1+\epsilon)$ for three different ϵ values. All three values of ν are much closer to 1, the Ising value, rather than to ∞, the KT value. Therefore, we believe that a nonzero anisotropy ($K\neq0$) makes the transition Ising-like.[11] To see physically why a KT-like transition is absent in our model after the Ising-like transition takes place, we plot in Fig. 2 the log of the vortex pair density as a function of $1/T$, the reciprocal of the temperature. The slope of this curve which is a measure of the chemical potential of a vortex-antivortex pair reduces drastically above T_c, similar to what happens in the isotropic XY model. This suggests that above the Ising transition, the effective V-A interaction is too weak to allow an intermediate XY-like phase.

To understand clearly what types of excitations destroy the long-range order, we have made a series of MC quench studies. At a temperature above the critical point,

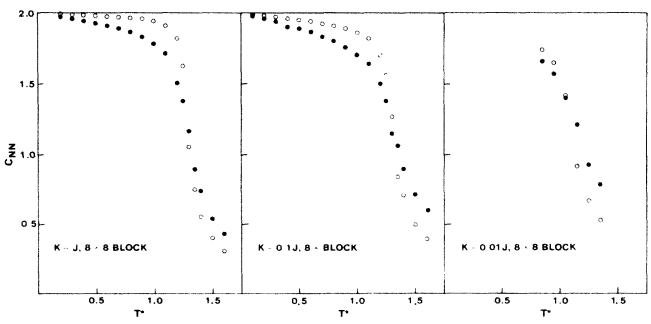

FIG. 1. Nearest-neighbor correlation as a function of T^* using MCRG analysis for $K/J=0.1$; 8×8 block spin lattices are matched starting from 16×16 and 32×32 lattices.

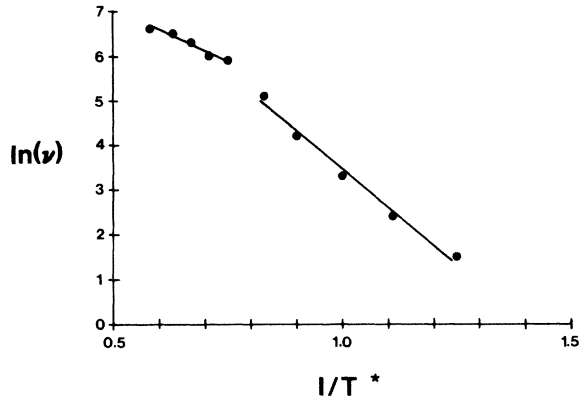

FIG. 2. Temperature dependence of the vortex-antivortex pair density.

the density of vortex pairs is considerably high. However, most of them have only a few MCS/s "lifetime." From a topological point of view, a tightly bound vortex pair is essentially different from an isolated vortex.[12] The former can annihilate each other by rearranging spins locally, but the effect of the latter in the system extends to any region no matter how far it is from the center of the vortex. Therefore, an isolated vortex, or a well-developed defect, would have a much longer MC lifetime in a quench process.

In Figs. 3(a)—3(d), we give our quench results starting from two initial temperatures $T > T_c$ and $T < T_c$. In both cases, the systems were quenched to $T = 0.1J/k_B$ and were monitored up to 2000 MCS/s after the quench. For the system quenched from $T < T_c$, the vortex-antivortex pairs annihilated each other after 50 MCS/s. In contrast, the quench from the high-T ($T > T_c$) phase shows drastically different behavior. In a few MC steps, again most of the closely spaced V-A pairs which are trapped inside wide domain walls annihilate each other, but after a long "time" one finds relatively long-lived defects consisting of V-A pairs connected by relatively sharp domain walls (strings[13] on the dual lattice). The total magnetization is still zero after 2000 MCS/s. This picture suggests that the LRO is destroyed by the formation of domains similar to the case of the 2D Ising system for which the wall tension vanishes at the transition temperature. Thus, our MKRG and MCRG results that the transition is Ising-like get further support from our quench study.

The particular type of long-lived defect structure that we see can be understood from a simple energy-entropy argument. The energy of a single vortex ΔE is found to be $\alpha J \ln N + 2KN$, where N is the number of spins and α is a constant. Thus, for a fully developed vortex, ΔE goes to infinity linearly with N in the thermodynamic limit as long as $K \neq 0$. However, the total energy of a V-A pair separated by a finite distance l is finite. We find the energy ΔE of a wall of width ω [see Fig. 3(a)] and unit length joining a vortex-antivortex pair to be

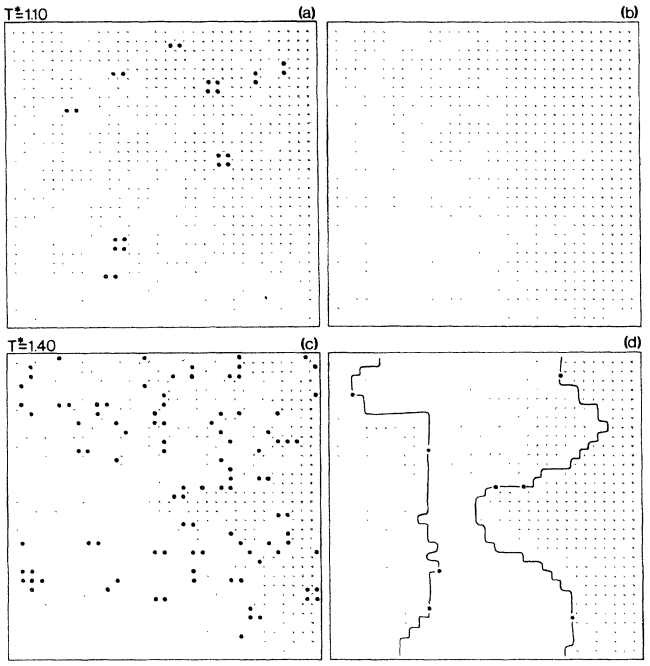

FIG. 3. Quenching studies starting from T_i to T_f (in units of J/k_B) for $K/J = 0.1$; ●=vortex and ○=antivortex. (a) $T_i = 1.1 < T_c$ (before quench), (b) $T_f = 0.1$ (50 MCS/s after quench), (c) $T_i = 1.4 > T_c$ (before quench), (d) $T_f = 0.1$ (50 MCS/s after quench).

$$\Delta E = \omega J \left[1 - \cos \frac{2\pi}{\omega} \right] + 2\omega K \ . \tag{4}$$

If $K = 0$, ΔE decreases continuously as $\omega \to \infty$, but if $K \neq 0$, the minimum of ΔE shifts to a finite ω; thus, the energy cost is linearly proportional to the separation of the V-A pair, instead of logarithmically as for the isotropic XY model. The entropy associated with the wall is also linear in l. Therefore, to minimize the free energy, it becomes favorable to produce these domain walls above a certain temperature and their floppiness (wall tension $\to 0$) is the reason for the phase transition. It is also the reason why the phase transition becomes Ising-like in the presence of anisotropy. We have shown two possible domain-wall configurations connecting a V-A pair in Figs. 4(a) and 4(b). The first one [4(a)] is discussed above and in the second [4(b)] the walls become thinner but the total-energy cost of the walls is same as in Fig. 4(a). Since the total wall length is now doubled, the second configuration has more entropy and is therefore expected to be formed more easily at high T. Figure 3 shows that this is indeed the case. In this configuration, the strings have a larger probability of meeting more vortices than one and it is indeed the case in our simulation.

To understand why a KT-like phase transition is absent in the present model we plot the log of the vortex pair density versus the reciprocal of temperature. We find that

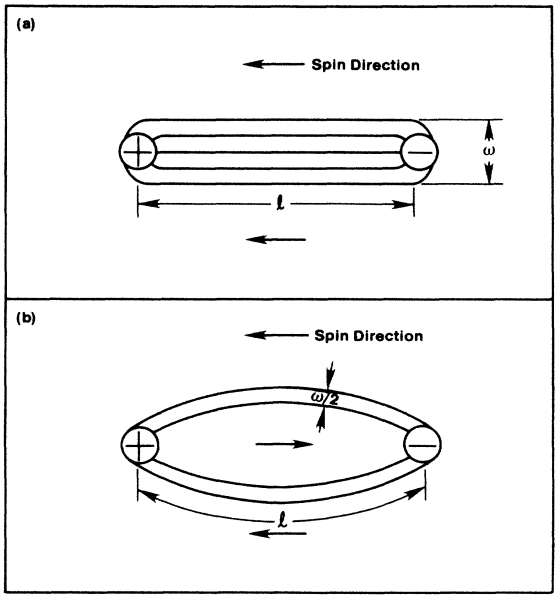

FIG. 4. Two possible vortex–domain-wall–antivortex configurations.

the chemical potential (μ) to produce a vortex pair reduces drastically at the transition temperature. This is similar to what happens at the KT transition temperature in the isotropic XY model.[9] We believe that above the Ising-like phase transition the effective V-A interaction is too weak to allow a XY-like phase.

In summary, we have found that in the presence of nonzero interaction anisotropy given by H of Eq. (2), the phase transition is Ising-like and the long-range order is destroyed by the formation of domain walls. Vortex and antivortex pairs tend to get trapped in the walls suggesting an attraction between these two types of excitations. Relatively long-lived excitations in this model are V-A pairs separated by domain walls of the type shown in Fig. 4(b). Our MC quench studies suggest that the nature of domain growth within the present model should be an interesting phenomenon to investigate. In particular, we propose to investigate the effect of domain-wall structure on domain growth kinetics, which is a subject of great current theoretical interest.[14]

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