Strings in Two-Dimensional Classical *XY* Models

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We study a class of simple, translationally invariant, two-dimensional, nearest-neighbor, isotropic *XY* models which possess, in addition to the familiar integer vortices, half-integer and "string" excitations. The half-integer vortices interact through both the logarithmic Coulomb potential and a linear potential mediated by the strings. The phase diagram of these models consists of three phases separated by lines of conventional Kosterlitz-Thouless transitions and lines of Ising transitions driven by the vanishing of the tension in the strings.

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In this Letter, we show that by modification of the cosine potential of the standard isotropic two-dimensional (2D) *XY* model one obtains an *XY* model which, in addition to the Kosterlitz-Thouless (KT) integer vortices,[1] exhibits extra topological excitations—half-integer vortices and "strings." The strings connect half-integer vortices and possess a "tension," i.e., mediate an effective interaction between half-integer vortices proportional to the distance between them. At the lowest temperatures this interaction binds the half-integer vortices together in pairs of integer vorticity; the low-temperature phase is therefore just that of the conventional *XY* model.[1] For appropriate parameter choices, however, the string tension can vanish as the temperature increases, which produces an Ising transition into a phase in which spins can flip by 180° with relative ease, but still exhibit a nonzero spin-wave stiffness at long wavelengths. A KT unbinding of the *half-integer* vortices restores the paramagnetic phase at a still higher temperature. In this case, therefore, the model has three phases. For other choices of parameters, the string tension remains finite at the half-integer KT temperature and therefore "confines" the half-integer vortices, preventing their dissociation. In this case, a single *integer* KT unbinding at a higher temperature restores the paramagnetic phase *directly,* and one obtains only the usual two phases.[2,3]

To illustrate this physics on a heuristic level, consider the following isotropic *XY* Hamiltonian:

$$\mathscr{H} = -\sum_{\langle rr'\rangle} [J\cos(2\delta_{rr'}) + \Delta\cos(\delta\theta_{rr'})]. \qquad (1)$$

Here r labels the sites of a square lattice, $\langle rr'\rangle$ represents nearest-neighbor pairs, $0 \leqslant \theta_r \leqslant 2\pi$ is the angle that the spin at site r makes with some fixed axis, and $\delta\theta_{rr'} \equiv \theta_r - \theta_{r'}$. For $\Delta \leqslant 4J$ the above potential has a metastable minimum at $\delta\theta = \pi$, which lies 2Δ in energy above the absolute minimum at $\delta\theta = 0$. Ising-type excitations of the perfectly ordered ferromagnetic ground state consisting of groups of spins overturned by 180° are then metastable. There are, in addition, excitations not present in Ising models, namely, one-dimensional strings of antiparallel spins that terminate in half-integer vortices and antivortices (Fig. 1). Such string excitations cost an energy equal to 2Δ times their length. That is, near $T=0$ the strings have a tension equal to 2Δ. The total energy cost of a half-integer vortex-antivortex pair separated by R is thus the sum of the usual Coulombic term,[1] roughly equal to $(2\pi/4)(\Delta + 4J)\ln R$, and a term roughly equal to $2\Delta R$ resulting from the string joining the vortices. (There is, of course, also an R-independent core energy of the vortices.) At low T there is insufficient thermal energy to create long strings, and so the half-integer vortices are bound together tightly in pairs. The many possible ways of connecting two half-integer vortices with a string give rise to a string "configurational" entropy proportional to R. Crudely speaking, then, the string tension decreases like $2\Delta - \alpha k_B T$ [$\alpha = O(1)$] with increasing T, vanishing at some critical temperature $k_B T_{c_1} = O(\Delta)$.

The phase diagram is determined by the relative magnitudes of T_{c_1} and the two other relevant temperatures in the problem, T_{c_2} and T_{c_3}, the half-integer and integer vortex-unbinding temperatures, respectively.

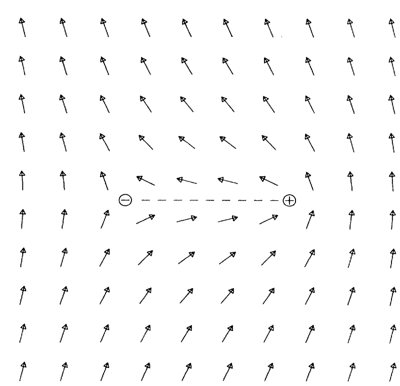

FIG. 1. A half-integer vortex-antivortex pair connected by a string. The centers of the half-integer vortices are represented by the circles around the plus and minus signs, and the string is represented by the dashed line.

Standard estimates[1] which ignore the strings give $k_B T_{c_2} = \frac{1}{8}\pi(\Delta+4J)$ and $k_B T_{c_3} = \frac{1}{2}\pi(\Delta+4J)$. The crucial point is that T_{c_1} can be varied independently of T_{c_2} and T_{c_3}. By adjusting the ratio Δ/J one can produce three possible scenarios.

(a) $T_{c_1} < T_{c_2} < T_{c_3}$. For $T < T_{c_1}$ one obtains the familar low-T phase of the XY model. At $T = T_{c_1}$ a phase transition, characterized by the vanishing of the string tension and hence of the free-energy cost to produce Ising excitations (i.e., spin flips) of infinite wavelength, occurs. The transition therefore belongs, whenever it is continuous, to the universality class of the Ising model. The spin-correlation function $g_1(r-r') \equiv \langle \exp[i(\theta_r - \theta_r')]\rangle$, which decays algebraically below T_{c_1}, decays exponentially, with the Ising correlation length, above T_{c_1}. Since for $T_{c_1} < T < T_{c_2}$ all half-integer and integer vortices remain bound in pairs, spin flips are the *only* excitations that disorder the system. Thus the algebraic decay of the correlation function $g_2(r-r') \equiv \langle \exp[2i(\theta_r - \theta_r')]\rangle$, which also measures orientational correlations but does not distinguish between the "head" and "tail" of a spin, persists in this temperature interval. At higher temperature, T_{c_2}, the system undergoes a KT transition wherein the half-integer vortices unbind, which produces the paramagnetic state characterized by exponential decays of both $g_1(r-r')$ and $g_2(r-r')$. Thus in this case there are three distinct phases.

(b) $T_{c_2} < T_{c_3} < T_{c_1}$. The half-integer–vortex pairs cannot unbind at T_{c_2}, but are confined in pairs by the positive string tension. Instead, at T_{c_3} the integer-vortex pairs, which are not bound by strings, dissociate, producing exponential decay in both $g_1(r-r')$ and $g_2(r-r')$ simultaneously.

(c) $T_{c_2} < T_{c_1} < T_{c_3}$. Again, at T_{c_2} the strings confine the half-integer vortices. As T approaches T_{c_1} from below, the half-integer vortex pairs become more and more loosely bound; eventually, at some critical temperature, T_c, bounded above by T_{c_1}, they screen the integer-vortex interactions sufficiently to induce an unbinding of the integer vortices, thereby restoring the paramagnetic phase. Just as for uniformly frustrated XY models,[3] it is not known whether the integer-vortex unbinding preempts or occurs simultaneously with the Ising transiton. In the latter case, the critical point presumably belongs in a new universality class which combines the logarithmic specific-heat singularity of the Ising model with the features of the KT transition. These features are illustrated in the schematic phase diagram of Fig. 2. Scenario (a) corresponds to moving along a curve which cuts through phases α, β, and $\mathscr{P}$ as T changes. Scenarios (b) and (c) correspond to a curve which cuts through α and $\mathscr{P}$ only.

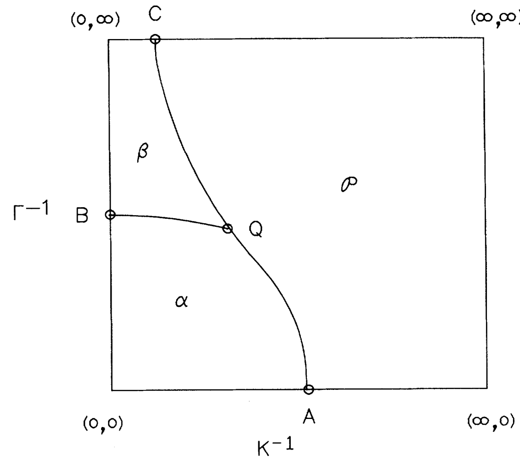

FIG. 2. Schematic phase diagram of the model defined by Eq. (2). In this diagram AQ, BQ, and CQ represent integer KT-type, Ising-type, and half-integer KT-type transitions, respectively.

Much of this physics can be obtained *analytically* from the following modified Villain-model[4] version of (1). The partition function of this model is

$$Z = \sum_{\{m_{rr'}\}} \prod_r \int_{-\pi}^{\pi} \frac{d\theta_r}{2\pi} \prod_{\langle rr'\rangle} \{\exp[-\tfrac{1}{2}K(\theta_r - \theta_{r'} - 2\pi m_{rr'})^2] + \exp[-\Gamma - \tfrac{1}{2}K(\theta_r - \theta_{r'} - \pi - 2\pi m_{rr'})^2]\}. \quad (2)$$

Here the $\{m_{rr'}\}$ are summed over all integer values; K and Γ are rough analogs of $(4J+\Delta)/T$ and Δ/T, respectively, in (1). [The usual Villain model[4] is given by (2) with $\Gamma = \infty$.] Performing standard duality transformations[5] on (2), one obtains

$$Z = \sum_{\{m_R\}} \prod_R \int_{-\infty}^{\infty} \frac{d\Psi_R}{2\pi} \exp\left(-\frac{K}{2}\sum_{\langle RR'\rangle}(\Psi_R - \Psi_{R'})^2 + i2\pi K \sum_R m_R \Psi_R\right) \prod_{\langle RR'\rangle} \{1 + \exp[-\Gamma - i\pi K(\Psi_R - \Psi_{R'})]\}. \quad (3)$$

Here R runs over the N sites of the dual lattice (which consists of sites situated at the centers of all elementary squares), and Ψ_R and m_R are the familiar[5] spin-wave amplitude and plaquette vorticity, respectively. If one expands the product

$$\prod_{\langle RR'\rangle} (1 + \exp\{-[\Gamma + i\pi K(\Psi_R - \Psi_{R'})]\})$$

in (3), there are 2^{2N} terms. It is simplest to represent each term of this expansion as a "bond graph," i.e., as a square array of lattice sites wherein some nearest-neighbor pairs are connected by a bond and the rest are not. In the bond graph representing any particular term of the expansion, a given pair $\langle RR'\rangle$ is connected if and only if, in the construction of the term, one has used the second summand in the curly brackets for that pair. Because each bond introduces a phase factor $\exp[-i\pi K(\Psi_R-\Psi_{R'})]$, the vorticity of any site R connected to an *odd* number of bonds is shifted by $\frac{1}{2}$, i.e., rather than being an integer m_R, it is of the form $m_R+\frac{1}{2}$. Any such site is occupied, in other words, by a half-integer vortex. Moreover, each half-integer vortex is connected to at least one other by a continuous chain of bonds: These are the strings.

Integrating out Ψ_R reduces (3) to $Z=Z_{\rm sw}Z_c$, where

$$Z_{\rm sw}=\prod_R\int_{-\infty}^{\infty}\frac{d\Psi_R}{2\pi}\exp\left(-\frac{K}{2}(\Psi_R-\Psi_{R'})^2\right),\quad Z_c=\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\{R_i\}}{}'C_{2n}(R_1,R_2,\ldots,R_{2n})Z_{2n}(R_1,R_2,\ldots,R_{2n}).\quad (4)$$

Here $Z_{\rm sw}$ is the spin-wave partition function, $\Sigma'_{\{R_i\}}$ denotes a sum over distinct $\{R_i\}$, i.e., those satisfying $R_1\neq R_2\neq\ldots\neq R_{2n}$, and $Z_{2n}(R_1,R_2,\ldots,R_{2n})$ is the usual Coulomb gas-partition function for a system with half-integer vortices situated at $\{R_1,R_2,\ldots,R_{2n}\}$:

$$Z_{2n}(\{R_i\})=\sum_{\{m_R\}}{}'\exp\left(\pi K\sum_{R\neq R'}(m_R+\nu_R)\ln\left|\frac{R-R'}{a}\right|(m_{R'}+\nu_{R'})+(\ln y_0)\sum_R(m_R+\nu_R)^2\right),\quad \nu_R\equiv\tfrac{1}{2}\sum_{i=1}^{2n}\delta_{R,R_i}.\quad (5)$$

Here the symbol $\Sigma'_{\{m_R\}}$ in (5) means a sum over all $\{m_R\}$ satisfying $\Sigma_R(m_R+\nu_R)=0$. $y_0=\exp(-\pi^2K/2)$ is the unrenormalized vortex fugacity. The quantity $C_{2n}(R_1,R_2,\ldots,R_{2n})$ is calculated according to the following graphical rules: Associate a Boltzman factor $e^{-\Gamma}$ with every bond; sum over all bond graphs in which every $R\in\{R_1,R_2,\ldots,R_{2n}\}$ is connected to an *odd* number of bonds, while all other dual-lattice sites are connected to *even* numbers of bonds. It is straightforward to prove that precisely these graphical rules are used[6] in the hyperbolic tangent expansion to compute the Ising $2n$-point correlation function for the nearest-neighbor reduced Ising Hamiltonian $\mathscr{H}_{\rm I}=-K_{\rm I}\Sigma_{\langle RR'\rangle}\sigma_R\sigma_{R'}$, where $\tanh(K_{\rm I})\equiv e^{-\Gamma}$. That is, $C_{2n}(\{R_i\})=\Lambda^{-1}Z_{\rm I}g_{\rm I}(\{R_i\})$, where $\Lambda=2^N\cosh^{2N}(K_{\rm I})$, and $Z_{\rm I}$ and $g_{\rm I}(R_1,R_2,\ldots,R_{2n})$ are, respectively, the Ising partition function and $2n$-point correlation function computed with $\mathscr{H}_{\rm I}$. Thus

$$Z_c=\frac{1}{\Lambda}Z_{\rm I}\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\{R_i\}}{}'g_{\rm I}(\{R_i\})\exp\left(\pi K\sum_{R\neq R'}(m_R+\nu_R)\ln\left|\frac{R-R'}{a}\right|(m_{R'}+\nu_{R'})+\ln y_0\sum_R(m_R+\nu_R)^2\right).\quad (6)$$

Equation (6) is the partition function for a system consisting of two kinds of vortices. The integer vortices interact through the usual Coulomb interaction; the half-integer vortices interact through both the Coulomb interaction and the potential $V_s(R-R')=-\ln g_{\rm I}(R-R')$, mediated by the string. Now let us examine the string potential in more detail. If $\Gamma\gg1$ (i.e., $K_{\rm I}\simeq0$), the associated Ising model is above its critical temperature. Its two-point correlation function $g_{\rm I}(R-R')$ therefore behaves like $\exp(-|R-R'|/\xi_{\rm I})$ for $|R-R'|\gg\xi_{\rm I}$. The string potential $V_s(R-R')$ is thus given by $\xi_{\rm I}^{-1}|R-R'|$, whereupon the string tension is just the inverse Ising correlation length, $1/\xi_{\rm I}$, and half-integer vortices are bound in pairs of integer vorticity and of typical linear size $\xi_{\rm I}$. On the other hand, if $\Gamma\simeq0$ (i.e., $K_{\rm I}\gg1$), $g_{\rm I}(R-R')\to M_0^2$, the square of the Ising magnetizaton, and the string tension vanishes. Clearly the critical value Γ_c (i.e., the temperature T_{c_1}) where the string tension first vanishes is determined by $\exp(-\Gamma_c)=\tanh(K_{\rm I}^{(c)})$, where $K_{\rm I}^{(c)}$ is the critical coupling of the Ising Hamiltonian $\mathscr{H}_{\rm I}$. If the string tension vanishes before any vortex unbinding occurs [scenario (a)] our model thus undergoes a transition in the Ising universality class.

To construct the phase diagram of (2) in (K,Γ) space, we first consider some limiting cases. When $\Gamma=\infty$, (2) reduces to the usual Villain model and therefore possesses an integer KT transition[4] (A in Fig. 2). When $\Gamma=0$, a change of variables from θ_r to $\phi_r\equiv2\theta_r$ transforms (2) into the partition function of the Villain model. However, because an integer vortex in the ϕ field is a half-integer vortex in the θ field, the phase transition (C in Fig. 2) corresponds to the unbinding of half-integer vortices. When $K=\infty$, the deviation in angle between nearest-neighbor spins is restricted to be 0 or π, with respective Boltzmann weights 1 and $e^{-\Gamma}$. In this limit (2) reduces to a nearest-neighbor Ising partition function with reduced exchange constant $K_{\rm I}'=\Gamma/2$. Note that in (6), which is the dual of (2), only the $n=0$ term contributes at $K=\infty$, so that $Z_c\sim Z_{\rm I}$. $K_{\rm I}'$ and $K_{\rm I}$ satisfy the duality relation $\tanh K_{\rm I}=\exp(-2K_{\rm I}')$.

Now let us consider small deviations from the limiting cases. When $\Gamma >> 1$, the Ising correlation length is $\xi_I \simeq 0$, so that only half-integer vortex pairs of small spatial extent ($\sim \xi_I$) occur. Since such tightly bound pairs do not influence the long-wavelength properties of the system, the phase transition remains integer-KT type in the neighborhood of A. [This is readily verified by a generalization to (6) of the Kosterlitz renormalization-group calculation.[1]] In the limit $1 << K < \infty$, the vortex fluctuations produce small perturbations in the Ising partition function Z_I. Expanding (6) as a series in y_0, we obtain, to lowest order,

$$Z \simeq \frac{1}{\Lambda} \sum_{\{\sigma_R\}} \exp\left(K_I \sum_{\langle RR' \rangle} \sigma_R \sigma_{R'} + \frac{y_0^2}{4} \sum_{R \neq R'} \left| \frac{R-R'}{a} \right|^{-\pi K/4} \sigma_R \sigma_{R'} \right). \tag{7}$$

Equation (7) is the partition function of an Ising model with algebraically decaying interactions. For sufficiently rapid decay, however, viz., for $\pi K/4 \geq 4$, such interactions are irrelevant to the critical behavior of the nearest-neighbor Ising model.[7] Thus the phase transition in the neighborhood of B remains in the universality class of the ordinary Ising model. Finally, when $\Gamma \simeq 0$, $g_I(R_1, R_2, \ldots, R_{2n}) \simeq M_0^{2n}$. Substituting this into (6) one can show that the main effect of the strings is to multiply the fugacity of the half-integer vortices by M_0. Since this trivial renormalization does not affect critical behavior, the half-integer KT transition persists in the neighborhood of C.

We have calculated the slopes of the phase boundaries at A, B, and C perturbatively. Combining these results with the earlier heuristic arguments, we arrive at the schematic phase diagram shown in Fig. 2. The three distinct phases in this figure are distinguished by the behavior of $g_1(r-r')$ and $g_2(r-r')$. In the phase labeled α, both $g_1(r-r')$ and $g_2(r-r')$ decay algebraically. In the phase labeled β, $g_2(r-r')$ decays algebraically and $g_1(r-r')$ decays exponentially. In the paramagnetic phase P, both $g_1(r-r')$ and $g_2(r-r')$ decay exponentially. Note that the nature of the phase diagram in the vicinity of the multicritical point, Q, in Fig. 2, is as yet unclear. In particular, the shapes of the phase boundaries near Q are unknown. Indeed, it is entirely possible that, e.g., the AQ boundary becomes a first-order line near Q. Similar uncertainties apply to BQ and CQ.

A physical realization of (1) or (2) is the isotropic-to-nematic phase transition in two-dimensional liquid-crystal systems in which the constituent long molecules have slightly different functional groups on the "head" and "tail" ends, and in which the interactions tend to align the heads of the molecules. For appropriate choices of Δ/J (or Γ/K) the system will first condense, as the temperature is lowered, into the ordinary nematic phase wherein the molecular axes align to produce quasi long-range orientational order, while the heads and tails of the molecules fluctuate randomly. Upon further cooling there will be a second Ising transition at which the heads and tails also align to establish quasi long-range order. In practice, other liquid-crystal transitions (e.g., the crystallization transition) may intervene before the Ising transition. The question of the existence of materials that do exhibit the two transitions is an interesting one.

The modified Villain model (2) is representative of the class of XY models characterized by nearest-neighbor interactions $U(\delta\theta)$ with *two* local minima in the range $0 \leq \delta\theta \leq 2\pi$. One could imagine a generalization to models whose nearest-neighbor potentials possess q local minima. The phase diagrams of these models probably consist of lines of KT transitions and transitions of a q-state model.[2]

The phenomena reported here are not unique to the 2D XY model. Any system with continuous symmetry and a potential with more than one minimum can, for appropriate parameters, acquire its fully ordered state via two successive transitions, one of which is Ising type. In particular, classes of three-dimensional XY and Heisenberg models will exhibit such behavior. There may be bulk liquid-crystal systems with distinguishable heads and tails that have, as in the two-dimensional case discussed above, two distinct nematic phases separated by an Ising transition.

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