Phase Diagrams of a Modified XY Model

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Much attention has been paid to the XY models from both theoretical and experimental perspectives. In two dimension, the system undergoes KT transition driven by the unbinding of thermally created topological defects[1]. A modified two-dimensional XY model is the system in which classical spins interact both ferromagnetically and nematically. Three phases occur as temperature and the interaction varied: a high-temperature disordered phase and two low-temperature phases algebraic correlations in, respectively, the ferromagnetic and nematic order parameters.

I. INTRODUCTION

A. The 2-dimensional XY model

The 2-dimensional XY model on the square lattice is defined by the Hamiltonian

$$H = -\sum_{\langle kl\rangle}[J_1 \cos(\theta_k - \theta_l)] \tag{1}$$

where the indices k and l numerate the lattice sites on a 2-dimensional square lattice, the sum is over the nearest-neighbour lattice sites and θ_k is the angle associated with each site which can take the values on the circumference. Variables θ_k can be thought of as the rotation angles of some planar magnetic moments with respect to a certain fixed direction.

The long-wavelength lattice waves are responsible for destroying the long-range order in the 2-D models[2]. Also Mermin and Wagner have proven that continuous global symmetries cannot break down spontaneously in systems with nearest-neighbor couping in two dimensions[3]. Nevertheless, there might exist a low-temperature phase with quasi-long-range order[1]. Kosterlitz and Thouless have shown that the model undergoes a Kosterlitz-Thouless (KT) phase transition from the quasi-ordered into a disordered high-temperature phase. The phase transition occurs at a temperature, when tightly bound topological defects (pairs of vortex and anti-vortex) unbind and become free.

B. High and low temperature regimes

In order to find statistical properties of the system, it is necessary to obtain an expression for the partition function and correlation functions. The partition function $\mathcal{Z}$ can be expanded as a high temperature series

$$\mathcal{Z} = \int_0^{2\pi} \frac{d\theta_0 \dots d\theta_n}{(2\pi)^n} \prod_{\langle kl\rangle}[1 + K\cos(\theta_k - \theta_l) + O(K^2)] \tag{2}$$

Similarly a high temperature expansion for the correlation function, $\langle \cos(\theta_0 - \theta_r)\rangle$ is constructed by adding $\cos(\theta_0 - \theta_r)$ to the Eqn 2. To the lowest order in K, each bond on the lattice contributes either a factor of one, or $\cos(\theta_k - \theta_l)$. Since,

$$\int_0^{2\pi} \frac{d\theta_i}{2\pi} \cos(\theta_i - \theta_j) = 0 \tag{3}$$

and

$$\int_0^{2\pi} \frac{d\theta_j}{2\pi} \cos(\theta_i - \theta_j)\cos(\theta_j - \theta_k) = \frac{\cos(\theta_i - \theta_k)}{2} \tag{4}$$

any graph with a single bond going out from an internal site vanishes. For the integral to produce a non-vanishing value, the integrand must reduce to a product of squares of cosines. To determine $\langle \cos(\theta_0 - \theta_r)\rangle$, we need to integrate over all terms which correspond to shortest path from site 0 to site r.

$$\begin{aligned}\langle \cos(\theta_0 - \theta_r)\rangle &= \int_0^{2\pi} \frac{d\theta_0 \dots d\theta_r}{(2\pi)^r} K\cos(\theta_0 - \theta_1) K\cos(\theta_1 - \theta_2) \\ &\dots K\cos(\theta_{r-1} - \theta_r)\cos(\theta_r - \theta_0) \\ &= K^r (\frac{1}{2})^{r-1} \int_0^{2\pi} \frac{d\theta_0 d\theta_r}{(2\pi)^2} \cos^2(\theta_r - \theta_0) \\ &\sim (\frac{K}{2})^r \sim e^{-\frac{r}{\xi}}\end{aligned}$$

where $\xi = \ln(2/k)$. We see that the correlation function diverges exponentially, since we are looking at the high temperature regime, corresponding to the disordered phase.

At low temperatures, θ_i varies slowly and smoothly throught the system. Then the cosine in the Hamiltonian can be expanded and only the quadratic term needs to be accounted for,

$$H = \int \frac{K}{2} d^d x (\nabla\theta)^2 \tag{5}$$

Then the correlation function can be found from Gaussian integration. Using standard rules of integration : $\langle e^A\rangle = e^{\langle A\rangle + \frac{1}{2}\langle A^2\rangle}$

$$\langle \cos(\theta_0 - \theta_r)\rangle = \langle \Re e^{i(\theta_0 - \theta_r)}\rangle = \Re exp[-\frac{1}{2}\langle(\theta_0 - \theta_r)^2\rangle]$$

The Gaussian averages, here, give the green's funtion $\langle \theta_{\vec{r}}\theta_0\rangle = G(\vec{r})$, where it satisfies

$$-\vec{\nabla}^2 G(\vec{r}) = \frac{1}{K}\delta^d(\vec{r}) \tag{6}$$

Using the gauss divergence theorem, we can take the integral. For d-dimensional system the integration gives us

$$\langle(\theta_0 - \theta_r)^2\rangle = \frac{2(r^{2-d} - a^{2-d})}{K(2-d)S_d} \quad (7)$$

where a is introduced to remove divergence for small length scales, and S_d denotes the d-dimensional solid angle, given as: $S_d = \frac{2\pi^{d/2}}{(\frac{d}{2}-1)!}$. For $d = 2$ we need the series expansion in Eqn. 7

$$[\frac{(r^{2-d} - a^{2-d})}{(2-d)}] \rightarrow [\ln r - \ln a] \quad (8)$$

Putting $d = 2$ for the solid angle, we obtain $S_d = \frac{2\pi}{(1-1)!} = 2\pi$. Hence

$$\frac{1}{2}\langle(\theta_0 - \theta_r)^2\rangle = \frac{1}{2\pi K}\ln\frac{r}{a} \quad (9)$$

Hence,

$$\langle\cos(\theta_0 - \theta_r)\rangle = (\frac{a}{r})^{\frac{1}{2\pi K}} \quad (10)$$

This equation indicates that correlation function, for a two dimensional XY model, decays as a power law. A power law decay usually denotes the existence of a phase transition that is associated with a critical point[4]. This is true for any spin system arranged on a two dimensional lattice, in the low temperature, Gaussian approximation. The low temperature phase of the XY model therefore is seen to behave like an ordered state, but we know that the correlation function decays as a power law. Hence this phase is described as a quasi long-range order state.

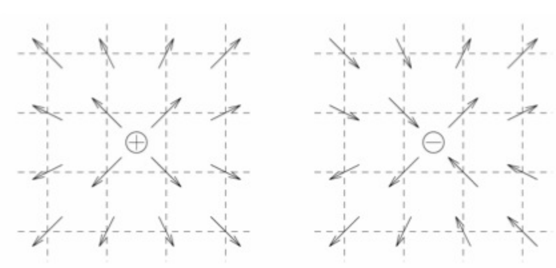

FIG. 1: Topological defects in the 2-D XY model with charge $n = +1$(left) and $n = -1$(right)[5].

J.M. Kosterlitz and D.J. Thouless suggested that the periodicity of the variable θ_i allowed for singular spin configurations -vortices- to appear in the system at sufficiently high temperatures, and they disorder the spin-spin correlation function[1]. The angle describing the orientation of a spin is undefined up to an integer multiple of 2π, the closed path integral of the gradient is $2\pi n$. As in FIG. 1 the integer n is the topological charge enclosed by the path.

At low temperatures, topological defects with the same magnitude and opposite sign can combine to form a dipole since the field caused by one charge will nearly be cancelled by the other charge with opposite sign, decreasing the overall energy cost of maintaining these defects. As the temperature of the system is raised, the size of the dipole grows and eventually, after a critical point, defects will behave as free particles forming a sea of charged defects.

II. MODIFIED XY MODEL

In this generalised two dimensional XY model, the classical spins interact with both ferromagnetic and nematic coupling. so the potential energy for a pair of spins has two minima as a function of their relative angle. At one minimum the spins are parallel; at the other they are antiparallel. The simplest Hamiltonian of this kind is

$$H = -\sum_{\langle kl\rangle}[\Delta\cos(\theta_k - \theta_l) + (1-\Delta)\cos 2(\theta_k - \theta_l)] \quad (11)$$

where θ_k, $0 \leq \theta_k < 2\pi$, indicates the spin orientation at site k, the summation is over nearest-neighbor pairs on a square lattice; Δ, $0 \leq \Delta \leq 1$, is the ferromagnetic coupling; and $1-\Delta$ is the nematic coupling. $\Delta = 1$ covers Kosterlitz and Thouless which results in spin waves and integer vortices. Domain walls and half-integer vortices control behavior near nematic limit, $\Delta \ll 1$[6]. When we increase Δ, half vortices are bound together, so that only integer vortices may exist freely. Thus here the model displays the KT transition.

As it is shown in Eqn. 13, for $\Delta < 1/5$ the intersite energy develops a metastable minimum at $|\theta_i - \theta_j| = \pi$. Pairs of half vortices are connected by a string where $\theta_i - \theta_j$ jumps by π and for $\Delta < 1$ this string has a finite tension.

$$\begin{aligned}\delta E(\alpha) &= \Delta\cos\alpha + (1-\Delta)\cos 2\alpha \\ \frac{d\delta E(\alpha)}{d\alpha} &= -\Delta\sin\alpha - 2(1-\Delta)\sin 2\alpha = 0 \quad (12)\\ \cos\alpha &= -\frac{\Delta}{4(1-\Delta)} \quad (13)\end{aligned}$$

The phase diagram for the modified XY model is constructed in FIG. 2, mainly by looking the behavior $T = 0$, $\Delta = 0$, and $\Delta = 1$[7]. To understand the nematic and ferromagnetic phases, we need to define two seperate correlation function and expect them to behave algebraicly. The first

$$G_1(r) = \langle\cos(\theta_0 - \theta_r)\rangle$$

is responsible for the ferromagnetic order. The second

$$G_2(r) = \langle\cos 2(\theta_0 - \theta_r)\rangle$$

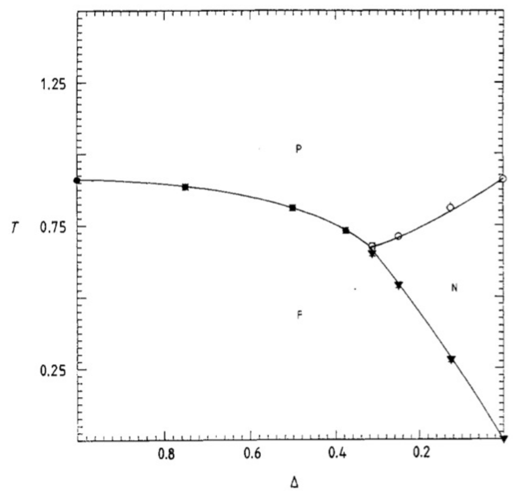

FIG. 2: The phase diagram for the modified XY model. The high-temperature disoirdered phase is denoted by P, the ferromagnetic phase by F and the nematic phase by N [6].

is responsible for both nematic and ferromagnetic order, in which spins have a axis but not unique direction. In high temperature phase they both should decay exponentially. In the ferromagnetic phase both quantities are expected to decay in algebraic order whereas in the low-temperature nematic phase $G_1(r)$ should decay exponentially and $G_2(r)$ algebraicly.

$$G_1(r) \sim r^{-\eta_1} \quad G_2(r) \sim r^{-\eta_2} \tag{14}$$

Close to the ferromagnetic line $(1 - \Delta \ll 1)$,one has essentially the conventional XY model. At low temperatures, spin waves destroy the long-range order of the ground state, leaving power-law decay of correlations. On the purely nematic-ferromagnetic line $T/\Delta = 5$, a modified version of this picture applies.

III. MONTE CARLO SIMULATION

The Metropolis algorithm[8] is used to get the simulation of the thermal equilibrium. This algorithm is shown to be ergodic and that new configurations are randomly generated. Each step in this algorithm is

1. Choosing randomly one site k of the lattice.
2. Choosing randomly an angle θ_k.
3. Calculating the energy difference ΔE_k between the actual energy and the energy if the spin at k is flipped around an axis defined by the angle θ_k.
4. If $\Delta E_k < 0$, then we accept the new configuration. Otherwise, we accept it with probability $\exp(-\Delta E_k / k_b T)$.

The simulation has been performed by D.B. Carpenter and J.T. Chalker to calculate the correlation functions $G_1(r)$ and $G_2(r)$ for various system sizes[6]. In FIG. 3, a configuration of the model is generated for $\Delta = 0.5$ that we can see the domain walls and linking pairs of half-integer vortices.

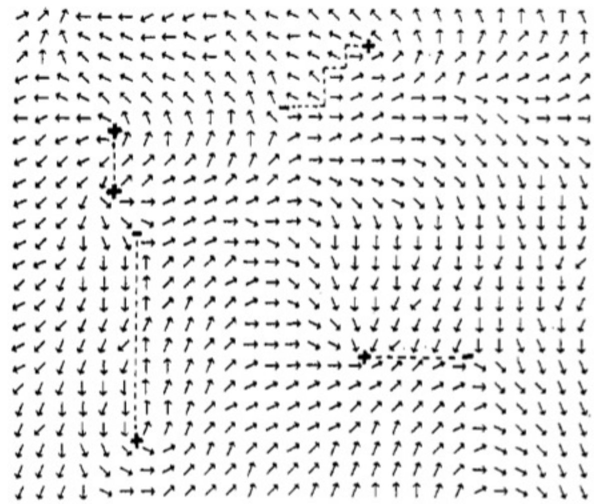

FIG. 3: A simulation generated from high temperature at $\Delta = 0.5$ where four domain walls are present and half-integer vortices are in linking pairs [6].

IV. CONCLUSION

The behavior of the XY model in low and high temperature regimes has been looked, where its asymptotic behavior in both the regimes turned out to be different, thereby indicating the existence of a phase transition between the high (disordered) and low (quasi-long range order) temperature phases. The peculiar nature of the disordering mechanism causing this phase transition, is that these disorders cannot be removed by any continuous transformations of the spin orientation. This led to accounting for the possibility of a new type defect in the XY model, known as the topological defect. The statistical mechanics of this generalised XY model is analysed mainly by considering the low-temperature behaviors. We construct phase boundaries that divide the phase diagram into three regions: XY-ferromagnetic, nematic and disoredered states. The Metropolis Algorithm is introduced for further simulations to get the detailied results.

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