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First-order transition in the XY model

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Recent Monte Carlo simulations suggest that changing the shape of the nearest-neighbor XY interaction might turn the infinite-order Kosterlitz-Thouless transition into a first-order one. In this Communication, an alternative explanation for the Monte Carlo data is proposed which is based on the renormalization pattern that results for this model in a Migdal-Kadanoff approximation.

It is well known that the conventional two-dimensional XY model shows an infinite-order transition from a low-temperature algebraic phase to a high-temperature paramagnetic phase. Two types of excitations are important at low temperatures: spin waves and vortices. The spin waves are responsible for the algebraic decay of the correlation functions in the low-temperature phase. The transition to the paramagnetic phase is brought about by the unbinding of pairs of vortices with opposite vorticity as first noted by Kosterlitz and Thouless.[1] This mechanism is confirmed by a renormalization-group analysis[2,3] of the XY model. The picture that arises from such an analysis is the following.[2-4] Under renormalization two things will happen: (i) The interaction shape, which is originally a pure cosine of the difference in angle of neighboring spins, changes and tends to become quadratic. (ii) The fugacity Z that controls the vortex density will start to decrease. The ultimate fate of a renormalization trajectory is governed by the Gaussian fixed line where the interaction is purely quadratic:

$$-\beta H_G = -\tfrac{1}{2} J_G \sum_{\langle i,j \rangle} (X_i - X_j)^2 \tag{1}$$

and $Z=0$, i.e., no vortices are present. It turns out[3] that the field Z is irrelevant only for $J_G > 2/\pi$; this means that only for low temperatures Z will continue to decrease and the trajectory will end up at the Gaussian fixed line that describes the algebraic phase. When the initial coupling is too small (i.e., temperature too high) the trajectory will be repelled from the Gaussian fixed line and end up at a high-temperature fixed point that corresponds to the paramagnetic phase. The separatrix between these two phases is the trajectory that ends at $J_{\mathrm{KT}} = 2/\pi$; the marginal eigenvalue present at this point is responsible for the infinite order of the Kosterlitz-Thouless (KT) transition.

In all of this the shape of the initial interaction does not seem to play a prominent role. The reason is that deviations from the quadratic shape are all irrelevant at the Gaussian fixed line. It is indeed a simple exercise in the evaluation of Gaussian correlations to check that the critical index of the eigenoperator that can be constructed from a perturbation of the potential of the form $V_{2m} = (X_i - X_j)^{2m}$ is given by

$$Y_{2m} = 2 - 2m \quad . \tag{2}$$

One expects therefore that not only the periodic (i.e., $Z=1$) model with a purely quadratic interaction (the so-called Villain[5] model) but also the conventional XY model with

$$-\beta H_{XY} = \sum_{\langle i,j \rangle} V(\theta_i - \theta_j) \quad ,$$
$$V(\theta) = J(\cos\theta - 1) \cong -\tfrac{1}{2} J \theta^2 \tag{3}$$

is described by the above picture.

It remains, however, an open question whether the same can be said for interactions with a shape that differs strongly from (2) or (3), as there might exist besides the Gaussian fixed line other fixed points in the function space of all possible interaction shapes. This question has been put again in the forefront by recent Monte Carlo results of Domany, Schick, and Swendsen[6] who study the possibility of generating a first-order transition in the XY model by a drastic change in the interaction shape. Their study is partly motivated by the fact that in the analogous problem of dislocation-mediated melting first-order transitions are commonly seen instead of the predicted KT transition.

Domany *et al.* consider a nearest-neighbor interaction

$$V(\theta) = 2J\{[\cos^2(\theta/2)]^{P^2} - 1\} \quad . \tag{4}$$

When P is large, this interaction is only approximately quadratic (with coupling strength JP^2) in a small region $|\theta| < \pi/P$ around the origin and exhibits a broad plateau for $|\theta| \geq \pi/P$. In contrast to the infinite-order KT transition expected for $P=1$, the Monte Carlo data for the energy per spin suggest[6] a first-order transition for $P^2 = 50$. In another Monte Carlo study for the same model van Himbergen[7] found that this transition is associated with a sudden increase in the number of vortex pairs in the system. These Monte Carlo results should, however, be considered with some caution for the following reason. If the orientations of the spins in the plane were not continuous but discrete i.e., $\theta = \pi l/P$, the model would have all the characteristics of a $2P$-state Potts model which is known[8] to have a first-order transition for $2P > 4$. In this case the change in nature of the transition is brought about by the fact that, in addition to the interaction shape V and the vortex fugacity Z mentioned above, a third parameter, namely, the field h_P conjugate to the operator $\cos(2\pi P\theta_i)$ (that tends to discretize the spins) plays an important role in the renormalization transformation. It is this field that becomes relevant[3] for low temperatures and hence destabilizes the Gaussian fixed line. Since the XY model (4) is continuous no such field is present in principle. However, in a Monte Carlo calculation that is carried out for a finite system there is clearly a minimal difference in angles needed to build vortices.

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The apparent discreteness brought into the problem in this manner might explain the first-order appearance of the Monte Carlo data.

In order to shed some light on this question I used the Migdal-Kadanoff renormalization[9] to investigate the possibility of new fixed points that could be responsible for the observed first-order transition. The Migdal-Kadanoff renormalization is known[3] to describe the KT transition relatively well. It constitutes a renormalization for the interaction shape only and is therefore well suited for the problem at hand. The fact that the vortex fugacity Z is not affected by the transformation has indeed the consequence that the Gaussian interaction is, strictly speaking, only approximately a fixed line of the transformation. But this does not constitute a real problem, neither in principle, as we know from other sources that Z renormalizes towards zero for low temperatures yielding a Gaussian fixed line even in the Migdal-Kadanoff approximation, nor in practice, as the Gaussian line is for $Z \neq 0$ numerically very stable in this approximation. The latter fact was recently again confirmed by Barber[10] who investigated the Migdal-Kadanoff renormalization for XY models with various initial interaction shapes. However, he did not explore the part of the function space with interaction shapes resembling those given by Eq. (4).

Instead of considering the Migdal-Kadanoff renormalization directly for the XY model it is more convenient to consider this transformation for the dual of this model which is a solid-on-solid (SOS) model.[3,11] (The actual Monte Carlo calculations of Domany *et al.*[6] were, in fact, also performed for this dual model.) Recall[3,11] that under duality the low-temperature algebraic phase of the XY model is mapped onto a high-temperature algebraic phase (the "rough" phase) of the SOS model while the high-temperature paramagentic phase of the XY model corresponds to the low-temperature "flat" phase of the SOS model. The periodic nature of the XY model is reflected by the fact that the statistical variables in the SOS model tend to take integer values. The role played by the vortex fugacity Z in the XY model is taken over by the field h_1 conjugate to the operator $\cos 2\pi X_i$. In particular, the XY model with full periodicity $(Z=1)$ corresponds to $h_1=\infty$, i.e., a pure SOS model with $X_i \equiv n_i$ and a nearest-neighbor interaction

$$-\beta H_{\mathrm{SOS}} = \sum_{\langle i,j \rangle} \phi(n_i - n_j) \tag{5}$$

given by

$$e^{\phi(n)} = \int_0^{2\pi} d\theta\, e^{V(\theta)+i\theta n} \Big/ \int_0^{2\pi} d\theta\, e^{V(\theta)} \ . \tag{6}$$

In general, both h_1 and ϕ will change under renormalization (see, e.g., Ref. 12) resulting in an attraction of the algebraic rough phase by the Gaussian fixed line $(h_1=0)$ when $J_G \leq \pi/2 = J_{\mathrm{KT}}^{-1}$.

In the Migdal-Kadanoff renormalization only the renormalization of ϕ is taken into account; it reads[3,9,10]

$$e^{\phi'(n)} = \sum_m \exp[2\phi(m) + 2\phi(m-n)] \Big/ \sum_m e^{4\phi(m)} \ . \tag{7}$$

Notice that this transformation applied to the continuous model $(h_1=0)$, where the sum is replaced by an integral, does not only have the Gaussian line as a fixed line but also reproduces exactly the indices (2) governing the stability against a change in shape. The transformation (7) has been studied for an initial interaction that has the characteristics of the dual of (4). Using (6) it is seen that the Boltzmann weights $e^{\phi(n)}$ for this model are unity for $n=0$, have a large almost constant plateau for $0 < |n| < P$, and have a oscillatory tail for larger values of n. Therefore the initial interaction is taken as

$$\begin{aligned} &\phi(0) = 0 \ , \\ &\phi(n) = -K, \quad 0 < |n| < P \ , \\ &\phi(n) = -\infty, \quad |n| \geq P \ . \end{aligned} \tag{8}$$

The renormalization trajectories resulting from (7) are given in Fig. 1 in a plot of $\phi^{(l)}(1)$ against $\phi^{(l)}(2)$ for the case $P=10$. The Gaussian axis is represented in this plot by the line $\phi(1)=\phi(2)/4$. It turns out that the high-temperature phase of the SOS model (i.e., points with initial values $K < 1.02$) streams, approximately along the line $\phi(1) = \phi(2)$, towards the Gaussian line at a much higher temperature $(J_G < 0.2)$. A slight decrease in temperature

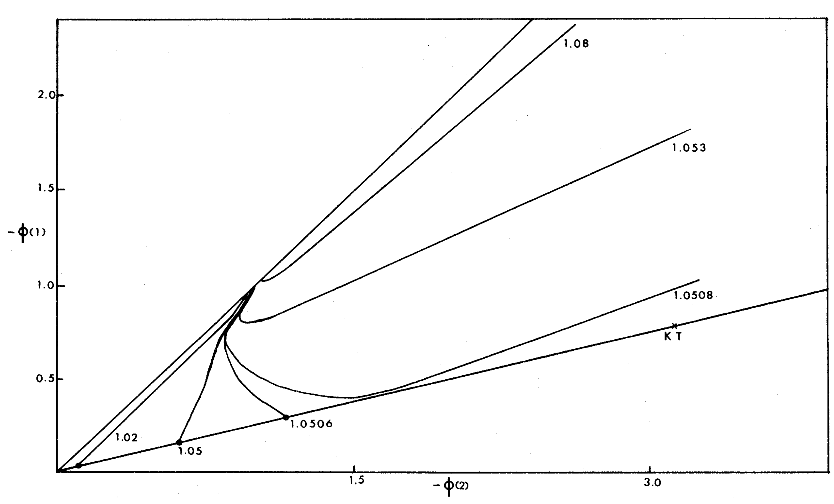

FIG. 1. Renormalization trajectories at various values of the initial coupling K. The straight lines with slopes 1 and $\frac{1}{4}$ represent the "Potts axis" and the Gaussian axis, respectively. The cross marks the location of the Kosterlitz-Thouless point.

results, however, in a stream in the opposite direction: all points with $K > 1.08$ are attracted by a low-temperature fixed point. On the face of it this behavior might be indicative for the observed first-order transition. It suggests the existence of a new non-Gaussian fixed point at $K \cong 1$ separating the algebraic high-temperature phase from the low-temperature phase. A closer study, however, shows that there is no true fixed point in this region of parameter space. The difference Δ between initial values and renormalized values defined as

$$\Delta^2 = \sum_n (e^{\phi'(n)} - e^{\phi(n)})^2 \tag{9}$$

exhibits merely a local minimum $\Delta \cong 0.06$ in this region of parameter space. Further, it turns out that the trajectories corresponding to initial values of K between 1.02 and 1.05 are still attracted to the Gaussian axis but at rapidly decreasing temperatures. The trajectory starting at $K = 1.0508$ passes close to the Kosterlitz-Thouless point $J_G = \pi/2$ (see Fig. 1).

These findings suggest a different explanation of the results seen in the Monte Carlo calculations[6,7] for this model. Due to the finite size of the systems considered, the Monte Carlo data corespond to only a few steps in a renormalization calculation. The point $K \cong 1$ might then still appear as a fixed point, generating an apparent singular structure corresponding to the spectrum of the linearized renormalization transformation in this region. The true asymptotic behavior is, however, governed by the KT point leading to an infinite-order transition. The distinction with the conventional XY model (or SOS model) is that in the present case the KT point is rapidly approached over a very small temperature range due to the action of the quasifixed point at $K \cong 1$. This also explains the rapid increase in the number of vortex pairs as seen by van Himbergen.[7]

In order to understand the origin of the quasifixed point at $K \cong 1$ it is instructive to consider the Kadanoff-Migdal renormalization for a $(2P-1)$-state Potts model. It is again given by Eq. (7) with the modification that the arguments of the functions ϕ are to be taken modulo $(2P-1)$. Inserting the initial interaction (8) leads in that case to a simple one-parameter recursion

$$e^{-K'} = \frac{2e^{2K} + 2P - 3}{e^{4K} + 2P - 2} \ . \tag{10}$$

This transformation has for $P = 10$ at $K \cong 1.15$ a fixed point that corresponds to the Potts critical point. The location of this fixed point, together with the fact that most trajectories for the SOS model (8) initially run along the Potts axis $\phi(1) = \phi(2)$, strongly suggest that the quasifixed point, that appears for the SOS model, is merely a remnant of the Potts fixed point. Since the Potts model undergoes a first-order transition this renormalization pattern leads to a different interpretation of the Monte Carlo data: an apparent first-order transition is suggested for small systems but the true asymptotic nature of the transition is still of the Kosterlitz-Thouless type.

Since the Migdal-Kadanoff renormalization used in this Rapid Communication is, of course, an approximation, the result obtained above is not yet conclusive but it shows at least a mechanism by which one can compromise the (apparent) first-order Monte Carlo data with a transition that is, in fact, of infinite order. Further research is required to see whether a similar mechanism can be at work in the case of dislocation-mediated melting.

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