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Berezinskii–Kosterlitz–Thouless transition close to the percolation threshold

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ABSTRACT

We use Monte Carlo to investigate the Berezinskii–Kosterlitz–Thouless transition close to the site percolation threshold in a square lattice. Several thermodynamic quantities are calculated for lattice sizes $L \times L$, from $16 < L < 640$. Our results are consistent with an infinite order transition for any value of the concentration of magnetic sites. We found that close to the critical percolation concentration, p_c (0.592746), the Berezinskii–Kosterlitz–Thouless transition temperature goes to zero as $T_{BKT} \propto (p - p_c)^{0.908}$ and the specific heat behaves as $T_{sh} \propto p^{1.133}$.

1. Introduction

Percolation in diluted models has been used as a prototype for a wide range of phenomena [1]. In particular, the effect of dilution in the phase transition in magnetic models is still a subject of interest in condensed matter physics [2–5]. Two-dimensional models with continuous variables are one of the most interesting magnetic models in physics [6]. They can present a non-usual infinite order phase transition with very interesting behavior [7,8]. Peculiar to this model is that a broken symmetry is not allowed [9] or, in other words, there is no an order parameter like the magnetization, $\mathcal{M}$, in an order–disorder phase transition. In spite of this lack of a genuine long range order, these systems can still have a phase transition mediated by the unbinding of point like defects. The transition is characterized by a qualitative change in the behavior of the correlation function, $G(r)$, of the wave function phase, the number density, the charge density or the spin component at site r of superfluid ^{4}He, two-dimensional crystalline solids, the two-dimensional Coulomb gas and the two-dimensional XY magnets respectively [1]. It is found that the correlation function decays as $G(r) \sim e^{-r/\xi(T)}$ at high temperature. The magnetic susceptibility is infinite at any temperature below T_{BKT}, the magnetization is zero at all temperatures and the specific heat is not critical. In contrast with the low temperature phase of a broken symmetry model where the correlation function decays to a constant value, in the *BKT* model the correlation function behaves as $G(r) \sim 1/r^{d-2+\eta}$. The exponent $\eta(T)$ is not universal depending continuously on temperature. In other words, there is a low temperature phase where the model is critical anywhere. In this Letter, we report a very careful numerical Monte Carlo calculation of the critical behavior of the *BKT* transition in a diluted model close to the percolation threshold. The simpler model belonging to this universality class is the classical two-dimensional XY model [6,10,11] defined by the Hamiltonian

$$H_{XY} = -J \sum_{\langle i,j \rangle} \epsilon_i \epsilon_j \left(S_i^x S_j^x + S_i^y S_j^y \right), \tag{1}$$

where $J > 0$ is an exchange ferromagnetic coupling nearest neighbors sites and ϵ_k assume the values 1 or 0 if the site is occupied by a magnetic or non-magnetic site respectively. The sum is over a $L \times L$ square lattice with periodic boundary conditions. The classical spin vector has three components, $\vec{S} = S^x\hat{x} + S^y\hat{y} + S^z\hat{z}$. In 1993 Lozovik and Pomirchi [12] reported some results for the Planar-Rotator model with bond dilution. They found that the *BKT* temperature behaves as $(\rho - \rho_c)^{1.55}$, were ρ is the density of magnetic bonds. This result agreed very well with an earlier paper by D.C. Harris et al. [13]. They found $(\rho - \rho_c)^{\nu}$, with $\nu = 1.56 \pm 024$. In a paper of 1996 Evertz and Landau [14] reported some results for the non-diluted version of this model using Monte Carlo and Spin dynamics techniques. They found $T_{BKT} = 0.700(1)$. More recently Leonel et al. [15] obtained the phase diagram $T_{BKT} \times p$ for the site diluted model. Here p is the fraction of magnetic sites in the system. The critical percolation concentration is $p_c = 0.592746$. They found that at $p = 0.7$, far above the percolation threshold, the *BKT* was extinguished. In 2003 Berche et al. [16] investigated the same model doing a more careful Monte Carlo simulation. They found that the apparent ill behavior of the system obtained by

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Leonel et al. [15] was a fake, probably due to a poor statistics. This was confirmed by other result [17]. More recently Young-Je et al. [18] measured the current–voltage characteristics of site-diluted Josephson-junction arrays. They found evidences that far below the percolation threshold the *BKT* transition is eliminated close to $p = 0.7$ and a different type of order is established. This result is in flagrant disagreement with Refs. [16,17].

2. Results

The main goal of this communication is to explore the *BKT* behavior of the system in a region close to the percolation threshold $p \approx p_c$. Before we proceed further some care must be taken. Close to p_c we expect that many non-percolating clusters appear in the system. Even closer to p_c it is possible that there will be no percolating cluster. When a percolating cluster appears its structure is fractal. All of this together makes the simulation close to p_c extremely difficult. Any cluster technique becomes useless here, since the cluster size is very small. Because of this we have used a simulated annealing [19] to reach the equilibrium in each simulation we did. Our simulations were performed in square lattices of dimensions $L \times L$ with $L = 10, 20, 40, 80, 160, 320, 640$. For the non-diluted model we went up to $L = 1280$. The result for $p = 1.00$ serves as a check for the correctness of our code. Each point in our simulation is the result of an average of over 10^8 up to 10^9 different configurations. In all cases the error bars are smaller than the symbol sizes when not shown.

In Monte Carlo simulations of the two-dimensional *XY* model it is possible to identify a magnetization since we deal with finite systems, however, as soon as $L \to \infty$, we obtain $\mathcal{M} \to 0$. As a characteristic of the model the specific heat has a non-divergent peak at a temperature dislocated above from T_{BKT}. The forth order Binder's cumulant, $U_4(L)$, that has a crossing at the critical temperature in an order–disorder model presents also problems to be applied in the present case. Since the model is critical in the entire region below T_{BKT}, we can expect that all curves U_4, for different values of L will coincide in this region as soon as L is large enough. In some simulations a crossing resembling an order–disorder transition can appear for small lattice sizes, but disappears as long as we increase the lattice sizes. Thus, magnetization, specific heat and cumulants are not reliable quantities to determine T_{BKT}. As pointed by Minnhagen [1] the behavior of the helicity modulus is the reliable quantity to be quested. Our decision of simulating so large lattice sizes is due to the dilution close to p_c. In this case, the percolating cluster has a small number of magnetic sites. (The maximum should be pL^2, when all sites are connected inside the percolating cluster.) This makes the system fluctuates wildly for $p \to p_c$ ($T_{BKT} \to 0$). The fluctuations can be smoothed by the use of large lattices. Another characteristics of the *BKT* transition is that the susceptibility, $\chi = \langle \mathcal{M}^2 \rangle$ behaves as $\chi \propto L^{\frac{7}{4}}$ at T_{BKT}. For large enough lattices that is a way to determine T_{BKT} and to characterize the transition. In Figs. 1 and 2 we show plots of $\chi \times T$ and $\Upsilon \times T$ for $p = 1$. The line $\Upsilon = \frac{2T}{\pi}$ intercepts the curves $\Upsilon(T)$ at T_{BKT} [1]. Using finite size scaling in both, Ξ and Υ the *BKT* temperature is determined as $T_{BKT} = 0.7001 \pm 0.0003$, consistent with earlier reports.

In Figs. 3 and 4 we show plots for the magnetization, $\mathcal{M}$, and Binder's cumulant, U_4, respectively, for $p = 0.600$ and several lattice sizes. The magnetization goes slowly to zero for large L as should be expected. The U_4 behavior shows the curves do not intercept at a common point as happens in the order–disorder phase transition, rather they share a common line as L grows. They separate apart as the *BKT* temperature is approached, $T_{BKT}(p = 0.600) \approx 0.02$ in this case.

Finally, in Fig. 5 we show a plot of T_{BKT} and T_{sh} (the maxima of specific heat) as a function of $(p - p_c)$. We adjusted a straight

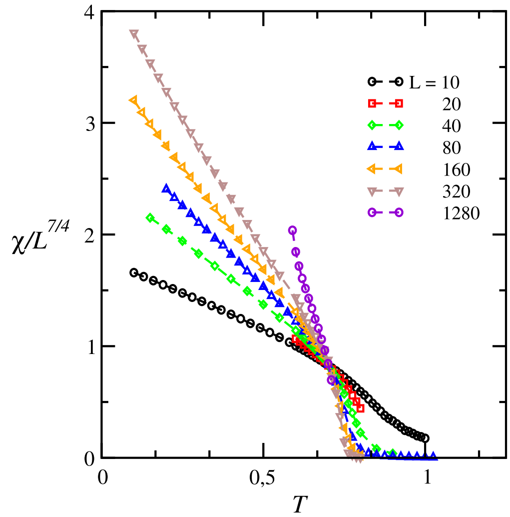

Fig. 1. In plane susceptibility Ξ times $L^{7/4}$ as a function of temperature for several lattice sizes as shown in the inset. Here we take $p = 1.00$. At T_{BKT}, Ξ scales as $L^{7/4}$ such that all curves should collapse at this point.

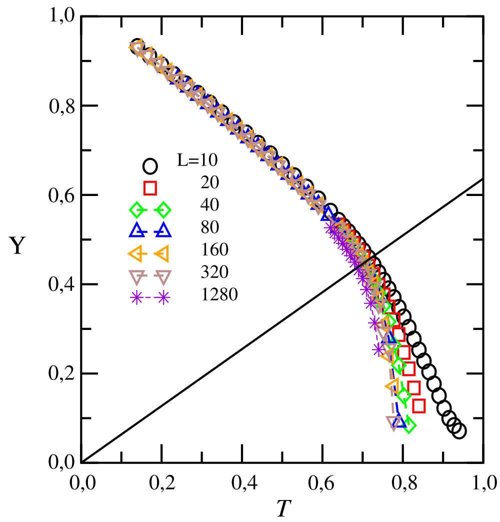

Fig. 2. The figure showns the helicity modulus for $p = 1.00$ as a function of temperature for several lattices. The straight line, $\Upsilon = \frac{2T}{\pi}$ intercepts the curves at T_{BKT}.

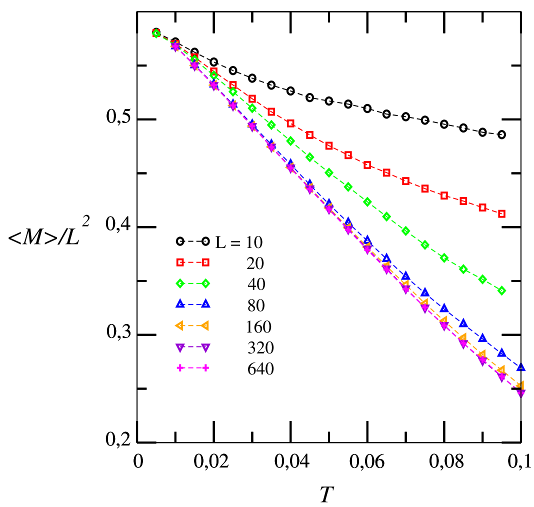

Fig. 3. The figure shows the finite size behavior of the magnetization for $p = 0.60$. The magnetization goes slowly to zero for large L as expected.

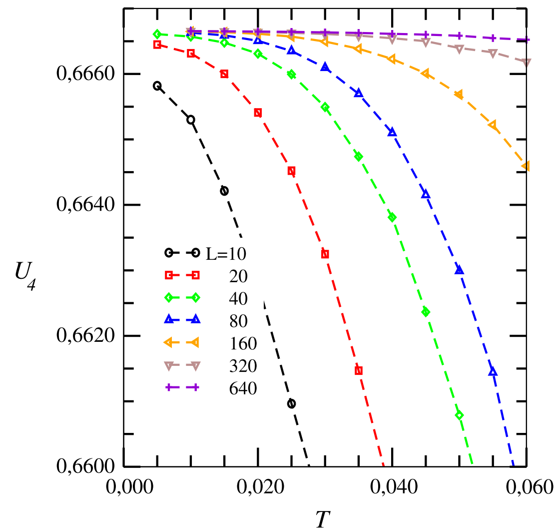

Fig. 4. A typical behavior of the Binder's cumulant, U_4 as a function of temperature and lattice size, L. Clearly, different curves for different values of L do not intercept themselves.

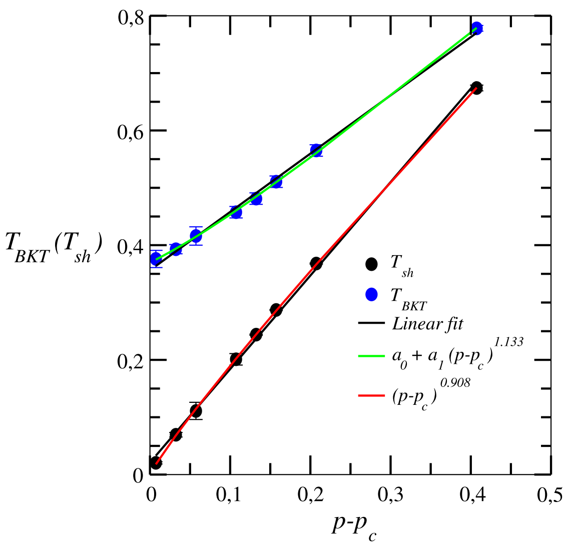

Fig. 5. Plot of T_{BKT} and the maxima of the specific heat, T_{sh}, as a function of $p - p_c$. Straight lines as well as power functions $(p - p_c)^q$ are adjusted to both curves. Clearly the power function adjusts much better to the simulated points than the straight lines. We have obtained $(p - p_c)^{1.133}$ and $(p - p_c)^{0.908}$ respectively.

line to both curves as well as a power function $(p - p_c)^q$. In both cases the power function adjusts much better to the simulated points than the straight lines. We have obtained $(p - p_c)^{1.133}$ and $(p - p_c)^{0.908}$.

3. Conclusions

Our results point in the direction that the *BKT* transition in the diluted two-dimensional *XY* model in a square lattice remains until the percolation threshold, when the *BKT* phase is extinguished. It seems that there is no any uncommon behavior in the classical model. Our hunch to the anomalous behavior obtained in Ref. [18] is that it was due to quantum fluctuations of the system. When the percolation threshold is approached, the *BKT* temperature goes to zero. In this regime, quantum fluctuations become important. Some very preliminary calculations using Stochastic Series Expansion [20] seems to give support to this. However, much work has to be done still, until we can have a more secure response to this.

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