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LETTER TO THE EDITOR

Binder's cumulant for the Kosterlitz–Thouless transition

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Abstract. It is shown that Binder's cumulant $U = 1 - \langle M^4\rangle / 3\langle M^2\rangle^2$ is very useful in the study of the Kosterlitz–Thouless transition of two-dimensional XY systems. It is possible to calculate the critical exponent η without knowledge of the critical temperature, and to exclude the possibility of a power law behaviour.

1. Introduction

The two-dimensional XY system has been the subject of extensive experimental, analytical, and numerical investigations [1]. Physically, the interest in this model arises from studies of thin films of liquid helium [2] or Josephson junction arrays [3].

Two-dimensional XY systems show a particular behaviour. The Mermin–Wagner theorem [4] proves that no magnetization appears at non-zero temperature (T). However, a Kosterlitz–Thouless (KT) transition [5] exists at the critical temperature $T_c \sim 0.9$, driven by the unbounding of vortex–antivortex pairs.

This transition has some special features: for $T < T_c$ the correlation length is infinite, while for $T > T_c$ it is exponential, decreasing contrary to the power law behaviour in the standard transition. These facts prevent the direct application of methods useful in the analysis of the standard transition and it is therefore difficult to obtain a clear result for the values of the critical temperature and exponent. A better method for obtaining a reliable T_c value is to use the helicity parameter, defined as the response of the system to a twist in one direction. This knowledge of the jump at the critical temperature allows one to obtain $T_c \sim 0.892$. However, in more complicated systems, such as frustrated systems (describing the Josephson junction array in a magnetic field), the jump of the helicity at the critical temperature is unknown and it would be very useful to obtain a method for obtaining T_c without using this jump. Moreover, the exponential behaviour in the KT transition has been questioned and a power law behaviour has been found in numerical simulations [6].

In this letter we will try to resolve these two questions. The method that is introduced is based on the Binder's cumulant $U = 1 - \langle M^4\rangle / 3\langle M^2\rangle^2$. This parameter has proved very useful for a standard power law transition and we will show that it is also useful in the case described here.

2. Model and algorithm

We choose for the classical $O(2)$ model an isotropic ferromagnet on a two-dimensional simple square lattice. The Hamiltonian for such spin system is given by:

$$H = J \sum_{(ij)} \mathbf{S}_i \,.\, \mathbf{S}_j \tag{1}$$

where $\mathbf{S}_i$ is a two-component classical vector of unit length and J is the ferromagnetic coupling constant ($J < 0$). We consider $L * L$ (L from 20 to 600) systems with nearest-neighbour interactions and periodic boundary conditions.

We use Wolff's single-cluster algorithm [7]. It has been demonstrated that this method is very effective in reducing critical slowing down for the $O(2)$ ferromagnetic spin model [8].

All simulations were carried out at temperatures where the finite size effects (FSS) are important: $0.89 < T < 0.92$ (for example, with size L =100 eight simulations at different temperatures were performed). In each simulation, at least 5 million measurements were made after enough single cluster updates (1 million) were carried out for equilibration. Note that our statistic is one order greater than that in previous studies [6].

We use in this work the histogram Monte Carlo technique developed by Ferrenberg and Swendsen [9, 10]. From a simulation done at T_0, this technique allows one to obtain thermodynamic quantities at T close to T_0. To obtain the quantities over the whole scale of temperatures we interpolate the results from different simulations by using smooth functions. Our errors are calculated with the help of the Jackknife procedure [11].

The quantities needed for our analysis in the FSS region are defined below. For each temperature we calculate:

$$\chi = \frac{N\langle M^2\rangle}{k_B T} \tag{2}$$

$$U = 1 - \frac{\langle M^4\rangle}{3\langle M^2\rangle^2} \tag{3}$$

where $\beta = 1/T$, M is the order parameter, χ the magnetic susceptibility per site, U is the fourth order Binder's cumulant [12] and $\langle \ldots \rangle$ means the thermal average. Note that the order parameter M is defined by the sum of all the spins.

3. Results

We concentrate first on the possibility of a power law behaviour for this system. This hypothesis has recently found some support [6]. In this case we can apply the standard laws for the FSS [13, 14]. In particular, to find T_c we can use the FSS of Binder's cumulant U. We record the variation of U with T for various system sizes and then locate the intersection of these curves. We compare the value of U for two different lattice sizes L and $L' = bL$, making use of the condition [12]

$$\left.\frac{U_{bL}}{U_L}\right|_{T=T_c} = 1. \tag{4}$$

In figure 1 U is plotted as function of the temperature for different sizes from $L = 60$ to $L = 600$. We notice that the curves cross each other; this is in conflict with the common belief for this model that the curves begin to separate at the critical temperature without crossing [15].

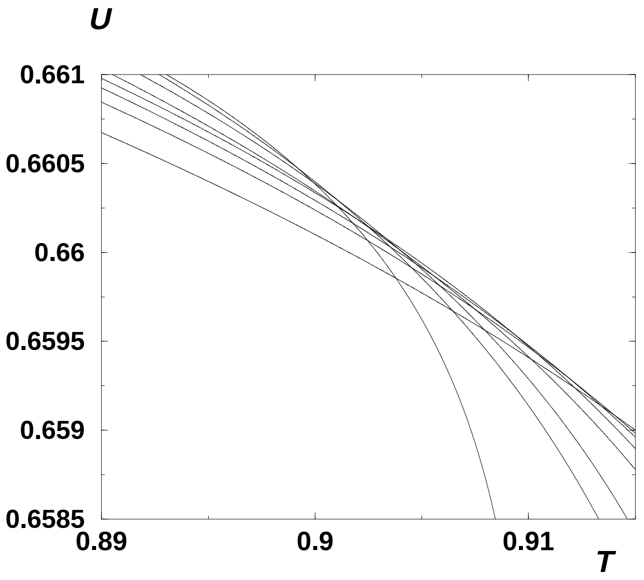

Figure 1. Binder's parameter U as function of the temperature for various values of L. In the left part of the figure, from bottom to top: $L = 40, 60, 80, 100, 150, 300, 400, 600$. For clarity, the values $L = 120$ and 200 are not shown.

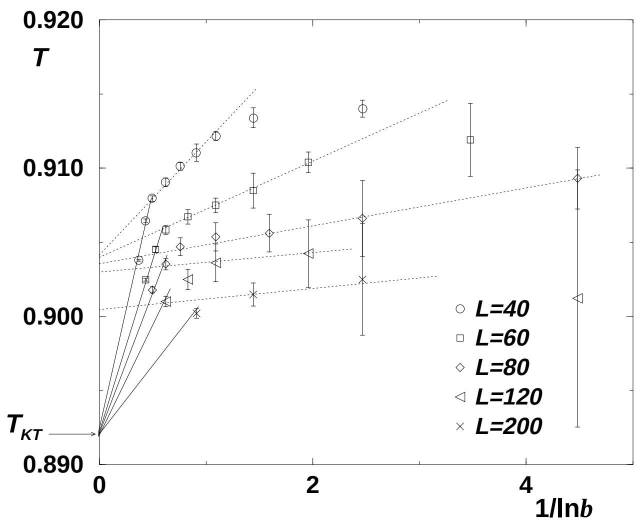

Figure 2. Crossing T plotted versus inverse logarithm of the scale factor $b = L'/L$. The results for $L = 40$, 60, 80, 120, 200 are shown. The estimated temperature $T_{KT} \sim 0.8921$ comes from [17].

Due to the presence of residual corrections to finite size scaling, one actually needs to extrapolate the results of this method for $(\ln b)^{-1} \to 0$. From this data we construct figure 2. This figure shows two different behaviours for each value. Firstly, for a value of b not too large the temperature of crossing seems to have a linear fit, but for large enough b the points show a 'crossover' to a new smaller critical temperature. For small lattices ($L < 100$) and small b the first linear curves (dashed line) converge to a critical temperature $T \sim 0.903$, and this could explain the numerical results in favour of a power law behaviour [6]. However, the 'crossover' which appears for all sizes excludes the possibility of a power law, even in presence of a strong correction. Moreover, the upper bound of critical temperature which we obtain ($T_c < 0.900$) does not agree with the result of high temperature expansion when a power law fit is used ($T_c \sim 0.930$) [16]. Our results are thus in favour of an exponential behaviour:

$$U(L,T) = f(L/\xi) + \text{corrections} \tag{5}$$

$$= f\{L \exp[c\,(T - T_c)^{\nu}]\} + \text{corrections} \tag{6}$$

where c is a constant, $\nu = 1/2$ and f is an unknown function. We have tried various fits to obtain the critical temperature found using the helicity $T_{KT} \sim 0.892$ [17], but the presence of the exponential (or logarithmic) form makes the fit useless and the only method that we are able to use is shown in figure 2; i.e., a linear fit when b is large enough. However, if our results are compatible with the exponential form and $T_{KT} = 0.892$, the critical temperature obtained by this fit can only give a rough estimate.

We concentrate now on the value of the critical exponent η. We can define it using a power law, valid whatever the form of ξ:

$$\chi = L^{2-\eta} g(L/\xi)\ . \tag{7}$$

To obtain η we can either use this formula at the critical temperature, where ξ is infinite, or try to plot $\chi\, L^{-(2-\eta)}$ as function of $g(L/\xi)$, where, obviously, ξ depends on T_c. Therefore, we have to know the value of T_c. This value is difficult to obtain for ferromagnetic systems (this work) and has been widely debated for the frustrated case (for example see [3]). We propose now a way to avoid this problem. The solution is to use the Binder cumulant U. In figures 3–5 we plot $\chi\, L^{-(2-\eta)}$ as function of U. Due to the form of U in (7) and neglecting corrections all sizes must coalesce in a single curve. The figures show our results for $\eta = 0.240$, 0.250 and 0.260. We observe that clearly the case 0.250 fits best. So we are able to obtain

$$\eta = 0.250(5) \tag{8}$$

compatible with the theoretical value $\eta = 0.25$.

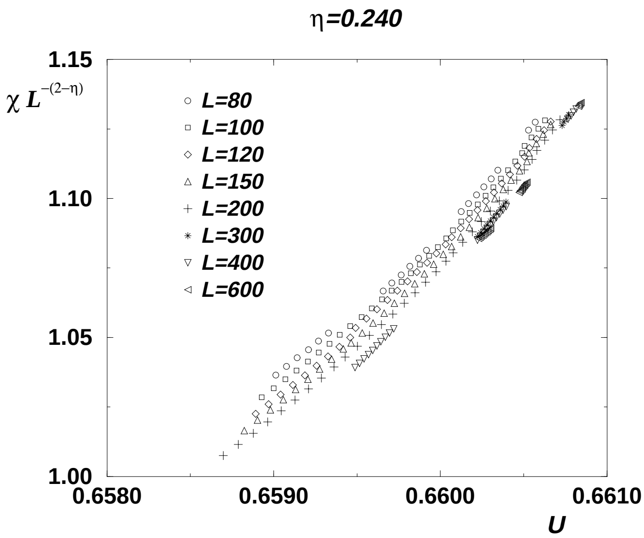

Figure 3. $\chi L^{-(2-\eta)}$ as function of U with $\eta = 0.240$ for the values $L = 80$–600.

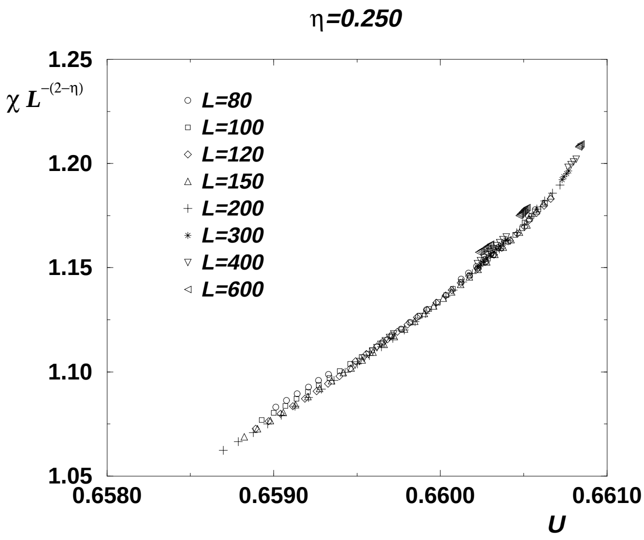

Figure 4. $\chi L^{-(2-\eta)}$ as function of U with $\eta = 0.250$ for the values $L = 80$–600. All the curves collapse to one. There is only one unknown parameter (η).

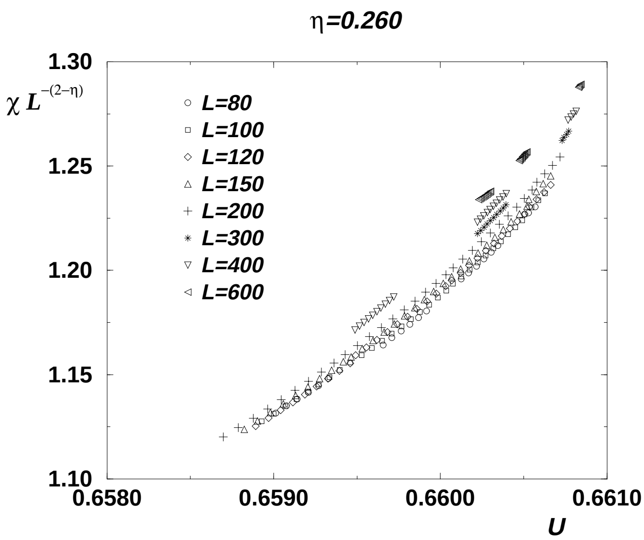

Figure 5. $\chi L^{-(2-\eta)}$ as function of U with $\eta = 0.260$ for the values $L = 80$–600.

4. Conclusion

We have shown that the use of the Binder cumulant is very useful in the study of the Kosterlitz–Thouless transition. Contrary to the common belief the cumulants cross for different sizes in the finite size region. Using this fact we are able to exclude the possibility of a power law behaviour for the transition and to give an upper bound for the critical temperature $T_c < 0.90$. Moreover, we are able to calculate the exponent η without knowledge of the critical temperature.

We have applied our scheme to the ferromagnetic system but it could be useful for the frustrated case corresponding to the experimental Josephson junction array in a magnetic field.

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