Dynamical phase transitions in the two-dimensional XY model

1989 J. Phys. A: Math. Gen. 22 L939

(http://iopscience.iop.org/0305-4470/22/19/004)

J. Phys. A: Math. Gen. 22 (1989) L939-L945. Printed in the UK

LETTER TO THE EDITOR

Dynamical phase transitions in the two-dimensional XY model

O Golinelli and B Derrida

Service de Physique Théorique de Saclay†, F-91191 Gif-sur-Yvette Cedex, France

Received 2 August 1989

Abstract. The 2D XY model is studied by Monte Carlo simulations where two configurations subjected to the same thermal noise are compared. We observe three temperature regimes: a high-temperature phase where the two configurations meet, an intermediate phase where they do not meet but their distance becomes independent of the initial distance, and a low-temperature phase where the distance remembers for very long the initial distance. The two transition temperatures $T_1 = 1.61 \pm 0.01$ and $T_2 = 0.95 \pm 0.05$ are estimated by means of finite-size scaling.

Since the discovery by Kosterlitz and Thouless (KT) of a phase transition in the two-dimensional XY model (Kosterlitz and Thouless 1973, Kosterlitz 1974), several numerical studies have tried to confirm the KT predictions and to estimate the transition temperature T_{KT}.

In most of the Monte Carlo simulations the susceptibility χ and the correlation length ξ (Tobochnik and Chester 1979, Gupta *et al* 1988), the magnetisation (Fernandez *et al* 1986) or the helicity modulus (Weber and Minnhagen 1988) were computed and the data were fitted assuming the singular behaviour predicted by the KT theory. According to these simulations,

$$T_{KT} \simeq 0.90.$$

Other approaches, based on approximate analytic methods (Mattis 1984) or on simulations done for a dual model, the SOS model (Shugard *et al* 1980) yield similar values for T_{KT}. However, it is usually hard to observe the KT transition directly without assuming the singular behaviour predicted by the KT theory.

In this letter, we try to extend to the 2D XY model a numerical method based on the comparison of two (or more) configurations subjected to the same thermal noise. This method has been already used for several systems, in particular for Ising ferromagnets (Derrida and Weisbuch 1987, Golinelli and Derrida 1988, Coniglio *et al* 1989) and for spin glasses.

In the case of Ising ferromagnets, two phases are observed: a high-temperature phase where the two configurations meet very quickly and a low-temperature phase where the two configurations never meet with a non-zero probability. It is possible to show (Lebowitz 1987, Neumann and Derrida 1988, Coniglio *et al* 1989) that these two dynamical phases coincide with the two equilibrium phases (in the paramagnetic phase, the two configurations evolve in the same valley and meet very quickly whereas in the ferromagnetic phase they can fall one in the + phase and the other in the −phase).

† Laboratoire de l'Institut de Recherche Fondamentale du Commissariat à l'Energie Atomique.

0305-4470/89/190939+07$02.50

In the case of the 3D spin glass, the dynamical phase diagram when comparing two configurations had more structure (Derrida and Weisbuch 1987). One could observe three phases separated by two transition temperatures T_1 and T_2. For $T > T_1$, the two configurations meet quickly. For $T_2 < T < T_1$, the two configurations never meet but their final distance is independent of their initial distance. For $T < T_2$, the two configurations do not meet and their distance presents memory effects, i.e. the distance remembers for very long the initial distance. This phase diagram resembles the diagram which was obtained by Ogielsky (1985) because T_1 and T_2 appear to be, respectively, close to the beginning of the Griffiths phase and of the spin-glass phase. However, up to now, one cannot exclude that these coincidences between the dynamical and the equilibrium phase transitions are accidental.

In the present work we consider the case of the 2D ferromagnetic XY model. We will see that the distance between two configurations has a behaviour which is very similar to the 3D spin glass showing three different phases. Using finite-size scaling arguments, we will estimate the transition temperatures T_1 and T_2 and we will see that the lower one is close to the Kosterlitz–Thouless temperature.

In our simulations, the classical spins are represented by an angle $\theta_i (0 \leq \theta_i \leq 2\pi)$. They are located on a square lattice of linear size L with periodic boundary conditions. The energy $\mathcal{H}(\mathscr{C})$ of a given configuration $\mathscr{C} = \{\theta_i\}$ is

$$\mathcal{H} = -\sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) \tag{1}$$

where the sum in (1) runs over all pairs of nearest neighbours on the lattice.

To make a configuration $\mathscr{C}(t) = \{\theta_i(t)\}$ evolve in time, we use the following Metropolis dynamics. During each time interval $\Delta t = 1/L^2$, we choose one site i at random among the L^2 sites and a random angle $\theta'(t)$ uniformly distributed between 0 and 2π. Let us call $\mathscr{C}'$, the configuration for which all angles are the same as in $\mathscr{C}(t)$ except that $\theta_i(t)$ has been replaced by $\theta'(t)$:

if $\mathcal{H}(\mathscr{C}') \leq \mathcal{H}(\mathscr{C})$ then $\mathscr{C}(t+\Delta t) = \mathscr{C}'$

if $\mathcal{H}(\mathscr{C}') > \mathcal{H}(\mathscr{C})$ then

$$\mathscr{C}(t+\Delta t) = \begin{cases} \mathscr{C}' \text{ with probability } \exp\left(\dfrac{\mathcal{H}(\mathscr{C}) - \mathcal{H}(\mathscr{C}')}{T}\right) \\ \mathscr{C}(T) \text{ with probability } 1 - \exp\left(\dfrac{\mathcal{H}(\mathscr{C}) - \mathcal{H}(\mathscr{C}')}{T}\right). \end{cases} \tag{2}$$

To implement these dynamics, a random number $0 \leq z(t) \leq 1$ is chosen and the configuration $\mathscr{C}'$ is accepted if $z(t) \leq \exp[(\mathcal{H}(\mathscr{C}) - \mathcal{H}(\mathscr{C}'))/T]$.

To compare two configurations $\mathscr{C}(t)$ and $\tilde{\mathscr{C}}(t)$ subjected to the same thermal noise, we choose at each time step the same site $i(t)$, the same angle $\theta'(t)$ and the same random number $z(t)$. Doing so, each configuration evolves according to the same Metropolis algorithm, but the two trajectories $\mathscr{C}(t)$ and $\tilde{\mathscr{C}}(t)$ are correlated: if they meet at time t ($\mathscr{C}(t) = \tilde{\mathscr{C}}(t)$), they remain identical for ever. To measure this correlation, we define the distance $D(t)$ between $\mathscr{C}(t)$ and $\tilde{\mathscr{C}}(t)$ to be

$$D(t) = \frac{1}{2L^2} \sum_i [1 - \cos(\theta_i(t) - \tilde{\theta}_i(t))]. \tag{3}$$

$D(t)$ depends on the system size L, the temperature T, the time t, the initial conditions $\mathscr{C}(0)$ and $\tilde{\mathscr{C}}(0)$ and the noise.

In the calculations which follow, we have averaged the distance over M samples. Since at a given time t, there are some samples for which $\mathscr{C}(t)$ and $\tilde{\mathscr{C}}(t)$ are still different and others for which $\mathscr{C}(t) = \tilde{\mathscr{C}}(t)$ implying that the distance is zero, we have averaged the distance $\langle D(t) \rangle$ over only those samples which have survived, i.e. such that $\mathscr{C}(t) \neq \tilde{\mathscr{C}}(t)$.

Figure 1 shows $\langle D(t) \rangle$ as function of the temperature T after 500 times steps ($t = 500$) for four choices of initial conditions.

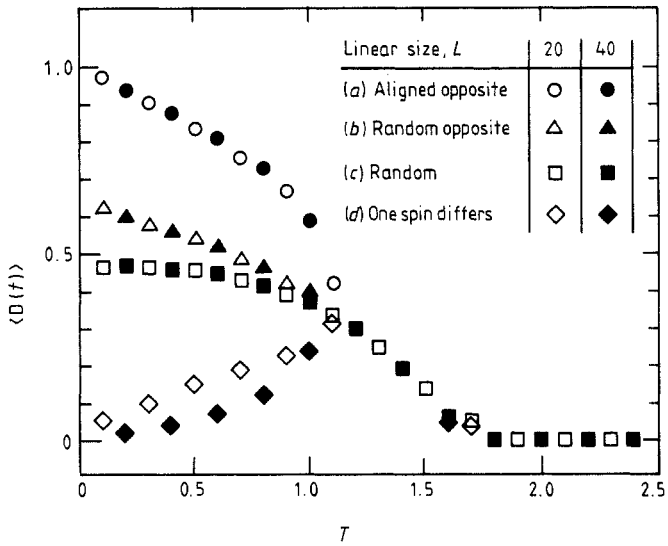

Figure 1. Distance $\langle D(t) \rangle$ as a function of temperature T after $t = 500$ time steps for the cases (a)-(d) as indicated on the figure and explained in the text. (Symbols are masked by the squares when they coincide.)

(a) $\mathscr{C}(0)$ and $\tilde{\mathscr{C}}(0)$ are aligned and opposite: $\theta_i(0) = 0$ and $\tilde{\theta}_i(0) = \pi$ for all i. So $D(0) = 1$ (circle symbols).

(b) $\mathscr{C}(0)$ is random and $\tilde{\mathscr{C}}(0)$ opposite: $\tilde{\theta}_i(0) = \theta_i(0) \pm \pi$ for all i. So $D(0) = 1$ (triangle symbols).

(c) $\mathscr{C}(0)$ and $\tilde{\mathscr{C}}(0)$ are random and independent. So $\langle D(0) \rangle = 1/2$ (square symbols).

(d) $\mathscr{C}(0)$ is random. $\tilde{\mathscr{C}}(0)$ is equal to $\mathscr{C}(0)$ for all sites except one, which is opposite. $D(0) = 1/L^2$ (diamond symbols).

Open symbols correspond to systems of linear size $L = 20$; for $L = 20$ the distance is averaged over 512 samples. Filled symbols correspond to $L = 40$, with 128 samples. The error bars are less than the size of symbols.

In case (d), where $D(0)$ is small, a large fraction of samples disappears in the first time steps. To keep the statistics of comparable quality, we averaged in case (d) over 1600 samples for $L = 20$ and 384 samples for $L = 40$.

We see in figure 1 three temperature regimes. For $T > T_1$ ($T_1 \sim 1.8$), the distance vanishes for all cases. In the range $T_2 < T < T_1$ ($T_2 \sim 1.2$), $D(t)$ does not vanish and does not depend on the initial conditions or on the system size. For $T < T_2$, $D(t)$ does not vanish and it depends on the initial conditions.

If one repeats the same calculations for other times in the same region, the results are similar. Except in the neighbourhood of T_2, the distances seem to have reached

their long-time limit. The comparison between full ($L = 40$) and open ($L = 20$) symbols shows that the results do not depend on the size, except for case (d) (because the initial distance $D(0) = 1/L^2$ depends on the size).

Therefore, as for the 3D spin-glass model, the XY model has an intermediate phase, where the distance reaches a non-zero equilibrium value, independent of the system size and of the initial condition.

Because the system is finite, two configurations will always meet. The difference between $T > T_1$ and $T < T_1$ is that the time for two configurations to meet for $T > T_1$ is small compared to 500 steps and for $T < T_1$ is large compared to 500 steps (for $T < T_1$ it increases quickly with the system size).

It is close to the temperatures T_1 and T_2 that the finite time and size effects are the most serious. This makes a precise determination of these temperatures difficult from the data of figure 1. To get a more reliable estimate of these transition temperatures we use a finite-size scaling method as in a previous work (Neumann and Derrida 1988).

For each sample s, we calculate the distance $D_s(t)$ defined by (3) at times $t = 1, 2, 3, \ldots$. The calculation can always be stopped when the distance vanishes since it remains zero at any later time.

Then we compute the following quantities:

$$\tau_1(L, T, s) = \sum_t t D_s(t) \left(\sum_t D_s(t) \right)^{-1} \tag{4}$$

$$\tau_2(L, T, s) = \sum_t t^2 D_s(t) \left(\sum_t D_s(t) \right)^{-1} \tag{5}$$

and the ratio

$$R(L, T, s) = \tau_2(L, T, s)/\tau_1^2(L, T, s). \tag{6}$$

τ_1 is a measure of a characteristic time for two configurations to meet and τ_2 is a measure of a characteristic squared time. They both depend on the size L, on the temperature T and on the sample s.

At the upper transition temperature T_1, one expects for τ_1 the following scaling form:

$$\tau_1(L, T, s) \sim u(L) f_1(v(L)(T - T_1), s) \tag{7}$$

valid for large L and T close to T_1.

$u(L)$ gives the size dependence at $T = T_1$ (for an ordinary second-order phase transition $u(L)$ and $v(L)$ are power laws). The symbol s means that τ_1 is sample dependent and the meaningful quantity to consider is the probability distribution of τ_1. One expects for τ_2 that

$$\tau_2(L, T, s) \sim u^2(L) f_2(v(L) T - T_1), s) \tag{8}$$

and since τ_2 is a measure of the squared characteristic time, one expects that the ratio τ_2/τ_1^2 should not depend on L at $T = T_1$:

$$R(L, T, s) \sim f_3(v(L)(T - T_1), s). \tag{9}$$

Averaging over many samples, one gets

$$\langle R(L, T, s) \rangle \sim g(v(L)(T - T_1)). \tag{10}$$

So we see that for large L, all the curves $\langle R \rangle$ plotted as functions of T should cross at the same temperature T_1.

In figure 2, we plot $\langle R\rangle$ averaged over 200 samples against the temperature T for several sizes ($L = 10$, 20 and 40). The errors bars are smaller than the sysmbols. The three curves cross at a temperature $T_1 = 1.61 \pm 0.1$.

Results of figure 2 were obtained using the initial conditions (b) ($\mathscr{C}(0)$ random and $\tilde{\mathscr{C}}(0)$ opposite). Other initial conditions would give different values of $\langle R\rangle$, but the estimate of the temperature T_1 would remain the same.

Let us now try to determine the temperature T_2 below which the distance after a long time depends on the initial distance. To do that we consider three configurations: $\mathscr{C}_1$, $\mathscr{C}_2$ and $\mathscr{C}_3$ subjected to the same thermal noise. $\mathscr{C}_1(0)$ and $\mathscr{C}_2(0)$ are randomly chosen and independent. $\mathscr{C}_3(0)$ is opposite to $\mathscr{C}_1(0)$. So the initial distances are different: $D_{12}(0) \simeq 1/2$, $D_{13}(0) = 1$ and $D_{23}(0) \simeq 1/2$. Then we measure $\Delta(t)$ defined by

$$\Delta(t) = D_{13}(t) - D_{12}(t). \tag{11}$$

$\Delta(t)$ plays the same role for T_2 as $D(t)$ for T_1. Above T_2, $\Delta(t)$ vanishes quickly whereas below T_2, Δ(t) does not vanish. The difference between $\Delta(t)$ and $D(t)$ is that when $D(t)$ vanishes, it remains zero for ever whereas $\Delta(t)$ has no reason for remaining zero after it has vanished for the first time. In order to keep the computation not too long, we measured $\Delta(t)$ at each Monte Carlo step and we stopped the calculation at the time τ when $\Delta(t)$ vanishes for the first time. τ_1, τ_2 and R were then computed with the new definitions:

$$\tau_n(L, T, s) = \sum_{t<\tau} t^n \Delta_s(t) \left(\sum_{t<\tau} \Delta_s(t) \right)^{-1} \tag{12}$$

$$R(L, T, s) = \tau_2(L, T, s)/\tau_1^2(L, T, s). \tag{13}$$

Thus τ_1 (and τ_2) is a measure of the characteristic (squared) time for the two distances D_{12} and D_{13} to become equal for the first time.

Above T_2, $D_{12}(t)$ and $D_{13}(t)$ quickly reach the same equilibrium value. Therefore τ_1 and τ_2 are short. In the low-temperature phase ($T < T_2$), the distance after a long

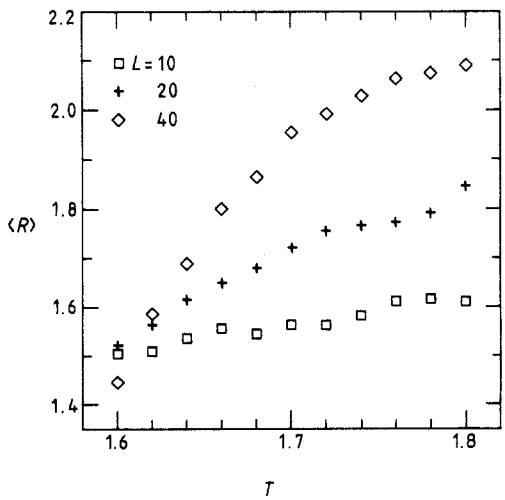

Figure 2. The ratio $\langle R\rangle = \langle \tau_2/\tau_1^2\rangle$ as a function at T for three sizes L. The curves cross at T_1.

time depends on the initial value for an infinite system. Because our simulations are done on finite systems, $\Delta(t)$ will always end up vanishing. However for $T < T_2$, τ_1 and τ_2 are very long.

On figure 3, we plot $\langle R \rangle$ averaged over 500 samples against T for $L = 10$, 20, 40 and 80. The curves cross at a temperature $T_2 = 0.95 \pm 0.05$. This gives an estimate for the temperature below which the distance depends on the initial distance.

This estimate for T_2 falls rather close to the Kosterlitz-Thouless transition T_{KT}. We have no proof that these two transition temperatures are the same. However, one can argue that below T_{KT} depending on the initial conditions, some defects might be trapped and that this would be responsible for the memory effects which are seen below T_2. It would, of course, be very interesting to improve the numerical data or to produce a better theoretical argument to decide whether T_2 coincides with T_{KT} because the same approach could be used for other systems (Barber and Derrida 1988).

Another question would be to know whether the dynamical transition at T_1 could be related to any equilibrium property of the system. A proposal has been made recently that T_1 could be due to the presence of a disorder point (Garel *et al* 1989). This disorder point would be related by the Coulomb gas transformation to the Hauge and Hemmer (1971) collapse transition at $T = 2T_{KT}$ of the neutral two-component Coulomb gas without hard core. However, no dynamical calculation has yet established the relation between T_1 and the disorder point and one cannot exclude that, as for the Heisenberg model (Martin 1985), the onset of instability at T_1 would be a pure dynamical effect.

In this letter we have seen that the distance between two configurations subjected to the same thermal noise has a very similar behaviour in the 2D ferromagnetic XY model and in the 3D spin glass. Three regimes exist and the low-temperature phase observed when one studies the distance seems to coincide with the low-temperature phase of the system at equilibrium. However, at the moment we cannot exclude that this coincidence is accidental.

We have also seen that one can use finite-size scaling ideas to locate the transition temperatures even in presence of memory effects. We think that one should be able

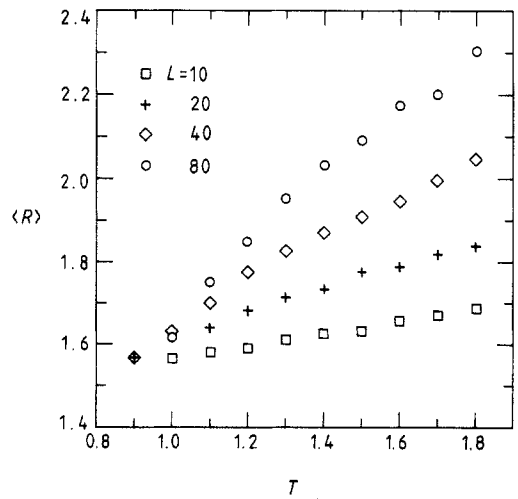

Figure 3. The ratio $\langle R \rangle$ computed with the difference of the distance ($\Delta = D_{13} - D_{12}$) as a function of T for four sizes L. The curves cross at T_2.

to use a similar approach to study remanence or aging effects which are present in spin glasses (Koper and Hilhorst 1988).

We would like to thank T Garel, H J Hilhorst, J Houlrik and J L Lebowitz for useful discussions.

References

Barber M N and Derrida B 1988 *J. Stat. Phys.* **51** 877
Coniglio A, de Arcangelis L, Herrmann H J and Jan N 1989 *Europhys. Lett.* **8** 315
Derrida B and Weisbuch G 1987 *Europhys. Lett.* **4** 657
Fernandez J F, Ferreira M F and Stankiewicz J 1986 *Phys. Rev.* B **34** 292
Garel, T, Niel J C and Orland H 1989 *Preprint*
Golinelli O and Derrida B 1988 *J. Physique* **49** 1663
Gupta R, Delapp J, Batrouni G G, Fox G C, Baillie C F and Apostolakis J 1988 *Phys. Rev. Lett.* **61** 1996
Hauge E H and Hemmer P C 1971 *Phys. Norvegica* **5** 209
Koper G J M and Hilhorst H J 1988 *J. Physique* **49** 429
Kosterlitz J M 1974 *J. Phys. C: Solid State Phys.* **7** 1046
Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181
Lebowitz J L 1987 private communication
Martin O 1985 *J. Stat. Phys.* **41** 249
Mattis D C 1984 *Phys. Lett.* **104A** 357
Neumann A U and Derrida B 1988 *J. Physique* **49** 1647
Ogielski A 1985 *Phys. Rev.* B **32** 7384
Shugard W J, Weeks J D and Gilmer G H 1980 *Phys. Rev.* B **21** 5309
Tobochnik J and Chester G V 1979 *Phys. Rev.* B **20** 3761
Weber H and Minnhagen P 1988 *Phys. Rev.* B **37** 5986