Frustration in two dimensions: phase transition for a Potts-XY model

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Abstract

We consider a Potts-XY model in two dimensions as a generalization of the Ising-XY model which described the Josephson-junction array under a magnetic field. We show that the transition is of first order and thus exclude for the present model the presence of a huge screening effect as it was emphasized in the Ising-XY case. We give some arguments that this conclusion holds for the latter case.

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I. INTRODUCTION

The nature of the phase transition in two dimensional frustrated XY systems like the Fully Frustrated lattice [1] or the triangular lattice [2] is still debated. A number of experimental systems are described by these models. For example the Josephson-junction array in magnetic fields (with a flux quantum per plaquette $f = 1/2$) [3–5], the superfluid transition of ^{3}He thick-films [6,7] or the surface phase transitions where the interplay between roughening and reconstruction of the surface is important (Restricted Solid On Solid model-RSOS) [8,9].

A very fascinating aspect of the thermodynamics of such systems is that they have two competing order parameters, the magnetization and the chirality (due to the non-collinear ground state), with two distinct symmetry groups, continuous $SO(2)$ rotations and discrete Z_2 lattice reflections, respectively. This has surprising consequences in view of Mermin-Wagner's theorem [10], which can be applied only in the first case ($SO(2)$) to show that the magnetization must vanish at any non zero temperature, according to the expected Berezinskii-Kosterlitz-Thouless [11] (KT) critical behavior associated with the rotation symmetry, while long-range order and an Ising-like phase transition are allowed for the chirality. However, in spite of twenty years of great effort [1–9,12–25] it is not clear whether the two transitions are distinct, with an intermediate phase, or if they are manifestations of a new universality class, in which the two transition temperatures could be melt in a single multicritical point. Monte Carlo results are in favor of two transitions at different temperatures with a new universality class associated to the Ising (chirality) symmetry ($\nu < 1$). However Olsson has claimed [12] that this behavior is due to a large screening length which prevents to reach the stable Ising fixed point ($\nu = 1$). In this interpretation, for a simulation with a system size larger than this screening length, the two transition will be decoupled and we observe first a standard transition of Kosterlitz-Thouless and then a standard Ising transition.

We generalized the breakdown of symmetry to $Z_q \otimes SO(2)$ where Z_q represent the Potts symmetry. For $q = 2$ we obtained the models discussed above. We therefore want to study the transition for $q \geq 3$. For ferromagnetic Potts model (Z_q symmetry alone), the transition is of second order for $q \leq 4$ and first order for $q > 4$ [26]. We have two objectives. Fist we want to have a better understanding of the the coupling between two symmetries without being restricted to the Ising-XY symmetries. Second we will show that the effect of the coupling with the $SO(2)$ symmetry is clearer for large q and that a first order transition appears for $q \geq 3$. This result will hold in the thermodynamic limit since a first order transition has a finite correlation length, therefore the two transitions must be coupled in this limit. This is in contradiction with Olsson's hypothesis for the case $q = 2$. In the conclusion we will argue that there is no fundamental differences between the case $q = 2$ and $q \geq 3$ and therefore the presence of a screening length in the Ising(q=2)-XY is not very plausible.

In section II we present the model. The simulations and the details of the finite size scaling analysis for a first order transition are explained in section III. The results are shown in section IV. Discussion and conclusions are in section V.

II. MODEL AND DETAIL OF THE SIMULATION

We consider the Hamiltonian on a square lattice:

$$H = -J_1 \sum_{(ij)} \mathbf{S}_i . \mathbf{S}_j . \delta_{q_i q_j} + J_2 \sum_{(ij)} \delta_{q_i q_j} \ , \tag{1}$$

where $\mathbf{S}_i$ are two component classical vectors of unit length, $\delta_{q_i q_j}$ are the three states Potts Hamiltonian ($q = 3$) with $\delta_{q_i q_j} = 0$ when $q_i \neq q_j$ and the interaction constant J_1 is taken positive. The sum runs over all nearest neighbor pairs (four in a square lattice). This Hamiltonian is the generalization of [13] where the Potts spins generalize Ising spins ($q = 2$).

The ground state (GS) depends on the value J_2/J_1. For $J_2 \leq J_1$ the GS is characterized by a ferromagnetic order for both XY spins and Potts spins. For $J_2 > J_1$ we obtain an antiferromagnetic Potts model and therefore no phase transition at temperatures different from zero [26,27].

The Hamiltonian (1) is a generalization of [13] but also very similar to the one of the Ashkin-Teller model [28] where two Ising models are coupled. In fact it belongs to a bigger class of models coupling two different transitions. Actually mainly Ising-Potts coupling [29] and Ising-XY coupling have been envisaged and this study can be seen as a step to enlarge the problem to more complicated systems.

The MC procedure is as follows. At each site one takes a new random orientation for the vector S_i and chooses a new random state for the Potts spin q_i. The interaction energy between this site and its neighbors is calculated. If it is lower than the energy of the old state, the new state is accepted. Otherwise, it is accepted only with a probability according to the standard Metropolis algorithm. Systems with $L = 20$, 40, 60, 80, 120, 150 have been simulated.

A. Definitions, histogram methods and finite-size scaling

We use in this work the histogram MC technique developed by Ferrenberg and Swendsen [30,31]. The histogram for the energy $P_T(E)$ is very useful for identifying a first order transition. Also the data obtained by simulation at T_0 can be used to obtain thermodynamic quantities at temperature T close to T_0. Since the energy spectrum of a Heisenberg spin system is continuous, the data list obtained from a simulation is basically a histogram with one entry per energy value. In order to use the histogram method efficiently, we divided the energy range $E < 0$ by 7 000 bins.

The critical slowing down in a first order transition (present for some values of J_2/J_1-see below) is greater than in a second order transition because of energy barriers, and thus the time of the simulation, to go from one state to another, grows exponentially with the size of the lattice. For this reason we have restricted our simulations to systems not too large to have satisfactory statistics. In each simulation, at least 13 millions measurements were made after enough Metropolis updating (1 million) were carried out to reach equilibration.

For each temperature T we have calculated the order parameter M (M_q) for the XY (Potts) spins by the sum of all the spins and the following quantities

$$C = \frac{< E^2 > - < E >^2}{N k_B T^2} , \tag{2}$$

$$V = 1 - \frac{< E^4 >}{3 < E^2 >^2} , \tag{3}$$

$$\chi_q = N \frac{< M_q^2 > - < M_q >^2}{k_B T} , \tag{4}$$

$$P_q = \frac{< M_q E >}{< M_q >} - < E > , \tag{5}$$

$$U_q = 1 - \frac{< M_q^4 >}{3 < M_q^2 >^2} , \tag{6}$$

$$U = 1 - \frac{< M^4 >}{3 < M^2 >^2} \tag{7}$$

where E is the energy, C the specific heat per site, V the fourth order energy cumulant, M_q is the Potts order parameter, χ_q the Potts magnetic susceptibility per site, P_q a cumulant, U and U_q the fourth order cumulant, $< ... >$ means the thermal average.

A large part of this work is devoted to the study of first order transitions which appear for certain values of J_2/J_1. To observe the nature of these transitions we will use the finite size scaling (FSS) theory [34–36]. A first order transition should be identified by the following properties:

a) $P_T(E)$ has a double peak.

b) The maximum of the specific heat C and the susceptibility χ_q and the cumulant P_q are proportional to the volume L^d.

c) The minimum of the fourth order energy cumulant V varies as:

$$V = V^* + b\,L^{-d}\ , \tag{8}$$

where V^* is different from $2/3$.

d) The temperatures $T(L)$ at which the quantities C, χ_q or P_q have a maximum should vary as:

$$T(L) = T_c + a\,L^{-d}. \tag{9}$$

III. RESULTS

A. $J_2/J_1 = 0$

We focus first on the case $J_2/J_1 = 0$. This is the closest form to the initial Ising-XY symmetry which appears in the two dimensional frustrated model or the superconductor.

In Fig. 1 the specific heat C is plotted as function of the temperature for various sizes (we note that the maximum is much larger than the usual value which is a sign of a first order transition). The value of the maximum as function of the volume is shown in Fig. 2 for C, χ_q and P_q. We note that the maxima vary like the volume except for the smaller sizes where further corrections are important.

In Fig. 3 we have plotted V as function of T for different sizes L. We can see that V does not tend to $2/3$ (for a second order transition) but to a value $V^* < 2/3$. This value is calculated by fitting the minimum with (8). As result we yield

$$V^* = 0.663(1)\ . \tag{10}$$

Fig. 4 shows the energy distribution for different sizes at different temperatures. The double peaks observed, even for a very small L, indicate a strong first order transition.

To obtain the critical temperature we can use (9). The result is

$$T_c = 1.1967(2)\ . \tag{11}$$

With this strong first order transition it is impossible to discriminate between the hypothesis of one or two transitions.

B. Phase diagram

We have performed many simulations in varying the value of J_2/J_1 to obtain the critical temperature T_c in Fig 5. In order to calculate the critical temperatures of the transitions associated to the $SO(2)$ symmetry (XY spins) and Z_3 symmetry (Potts spins) when they are decoupled, we use the Binder's cumulants. 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 [32]

$$\left.\frac{U_{bL}}{U_L}\right|_{T=T_c} = 1. \tag{12}$$

We have proved that this method, introduced for the standard transition (similar to Potts type), works also in the case of a Kosterlitz-Thouless transition ($SO(2)$ symmetry) [33] contrary to the common belief of a merge of the curve at the critical temperature.

We have three different properties of the model depending on J_2/J_1.

a. For $J_2/J_1 > 1$ no phase transition appears at non zero temperature. Indeed with this value and the Hamiltonian (1), the interactions between the Potts spins are antiferromagnetic. In this case we know that the system is disordered for $T > 0$ [26,27].

b. For $-0.4 \lesssim J_2/J_1 < 1$ a first order transition exists.

c. For $J_2/J_1 \lesssim -0.4$ two transitions appear, associated to the XY symmetry at low temperature (ferromagnetic Kosterlitz-Thouless transition) followed by the transition associated to the Potts symmetry (ferromagnetic three states Potts transition).

This phase diagram is similar to those obtained by Granato et al [13] for $q = 2$ except for transitions on the line PD which is of second order in the Ising-XY case.

For larger $q \geq 4$ we obtain similar phase diagrams as for $q = 3$.

IV. DISCUSSION AND CONCLUSION

We have studied in this work the phase transition for a breakdown of symmetry of the type $SO(2) \otimes Z_q$ for $q \geq 3$. We obtained the phase diagram for general J_2/J_1 (see Hamiltonian (1)) and in particular a first order transition for $J_2/J_1 = 0$ which is the model related to the Fully Frustrated XY model [13]. Thus the coupling of the XY symmetry $SO(2)$ with the Potts symmetry Z_q has the tendency to lower the value q from which a first order transition appears ($q > 4$ for a Z_q symmetry alone).

Since the correlation length is finite for a first order transition and also is visible for the lattices we simulate the transition in the thermodynamic limit (infinite size) should be as well of first order. Therefore in this limit the two symmetries will be coupled. This fact excludes the presence of a "screening length" in our model ($q \geq 3$) which could prevent for lattices accessible in numerical simulation the "true" decoupled behavior as claimed by Olsson [12] for the $q = 2$ case.

The question now is how we can apply our results obtained for $q \geq 3$ to the Ising case $q = 2$. First we note that the Hamiltonian (1) is ferromagnetic in the sense that there is only one ground state and therefore no entropy at $T = 0$. In this case we know that there is no fundamental differences between the Ising symmetry ($q = 2$) and the $q = 3$ Potts model when there are not coupled to the XY symmetry. The same formalism applies and only the critical exponents are different. The only difference between the two model appears in presence of disorder. The ferromagnetic Ising fixed point is stable contrary to the three state Potts fixed point [37]. However we do not think that it applies to our case. Therefore this work suggests by similarity of the Potts($q = 3$)-XY case that there is no "screening length" in the Ising-XY model and then the transition belongs to a new universality class with $\nu < 1$.

In conclusion we have shown that the coupling between a Potts symmetry with $q \geq 3$ with a $SO(2)$ (XY) symmetry lead to an unambiguous first order transition, i.e a coupled transition. We have given some arguments which show that this last conclusion could be applied in the Ising-XY coupling.

V. ACKNOWLEDGMENTS

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FIGURE CAPTIONS

Fig. 1: Specific heat for various sizes as function of the temperature.

Fig. 2: Maxima of the specific heat C, the susceptibility χ_q and P_q in function of the volume $L^2 \cdot L_z$ for the STAR model.

Fig. 3: V as function of the temperature for different sizes. The dashed line indicates the value of $V^* = 2/3$ for a second order transition. The broken line is our estimate of $V^* = 0.663(1)$ at the critical temperature $T_c = 1.1697$.

Fig. 4: Energy histogram $P(E)$ as function of energy per site E for various sizes L at different temperatures of simulation: $T_{20} = 1.2095$, $T_{40} = 1.2004$, $T_{60} = 1.1985$, $T_{80} = 1.1973$, $T_{120} = 1.1970$, $T_{150} = 1.19693$.

Fig. 5: Phase diagram for the Potts–XY (q=3) model in two dimensions. The case $J_2 = 0$ (section III A) is shown by a black circle. Solid and dotted lines indicate continuous and first-order transitions respectively.

FIGURES

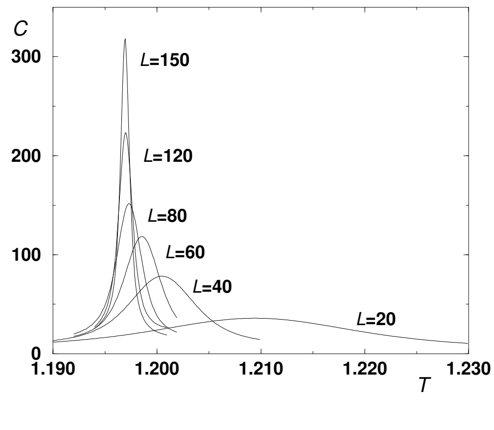
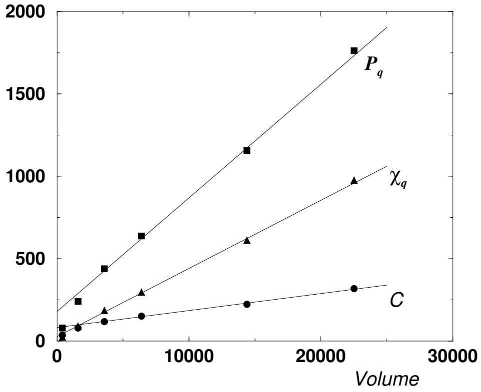


FIG. 1.



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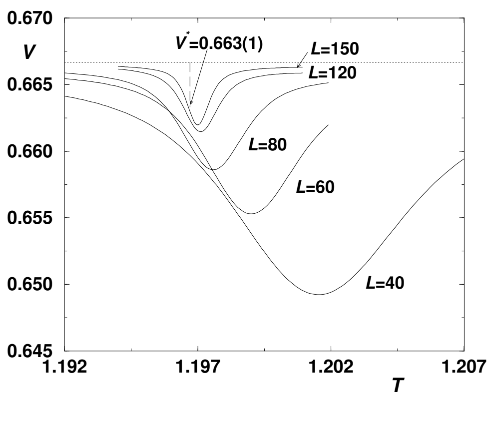

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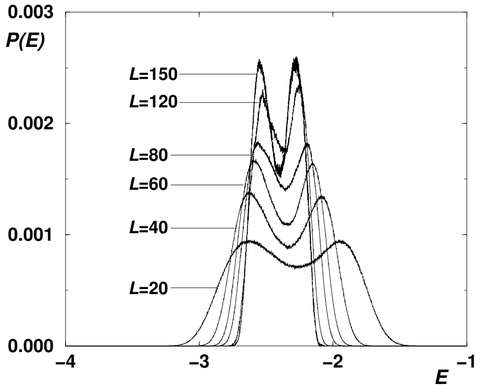

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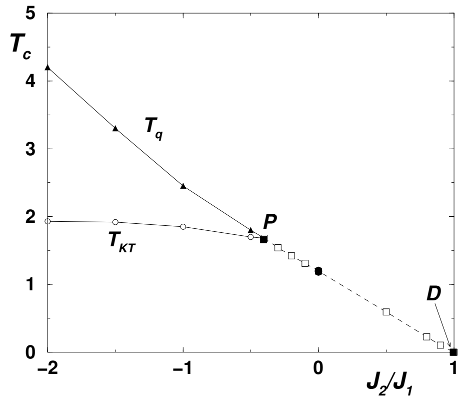

FIG. 5.