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Monte Carlo study of 2D generalized XY-models

L.A.S. Mól[1,2], A.R. Pereira[2,a], H. Chamati[3,b], and S. Romano[3]

[1] Departamento de Física, Universidade Federal de Minas Gerais, Caixa Postal 702, 30123-970, Minas Gerais, Brazil
[2] Departamento de Física, Universidade Federal de Viçosa, Viçosa, 36570-000, Minas Gerais, Brazil
[3] Istituto Nazionale per la Fisica della Materia e Dipartimento di Fisica "A. Volta", Universitá di Pavia, via A. Bassi 6, 27100 Pavia, Italy

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Abstract. In this paper we study a recent generalization of the XY-model in two dimensions by using Monte Carlo method. The vortex density, specific heat, energy and critical temperature are obtained. Some results are compared with approximated analytical calculations. The nature of the phase transition as the generalization parameter varies is discussed.

PACS. 05.50+q Lattice theory and statistics – 75.10.Hk Classical spin models – 75.40.Mg Numerical simulation studies

1 Introduction

One of the simplest models supporting topological excitations in the spin field is the two-dimensional (2D) planar rotator model $H = -J\sum_{i,j}(S_i^x S_j^x + S_i^y S_j^y) = -J\sum_{i,j}\cos(\phi_i - \phi_j)$, where $J > 0$ is the ferromagnetic coupling constant, ϕ_i are the angular coordinates of spins $\vec{S}_i = (S_i^x, S_i^y) = (\cos\phi_i, \sin\phi_i)$ and i, j indicate nearest neighbor sites of a $L \times L$ square lattice. It is well known that this model exhibits the Berezinskii-Kosterlitz-Thouless (BKT) phase transition [1–3] at a temperature T_{BKT} due to unbinding of vortices. Generalizations of this model have also attracted much interest in the two last decades, mainly in connection with the nature of the phase transitions. Such generalizations can be written as $H_{gpr} = -\Sigma_{i,j}V(\phi_i - \phi_j) = -\sum_{i,j}V(\Phi)$, where $\Phi = \phi_i - \phi_j$. Domany et al. [4] have considered a generalization of the form $V(\Phi) = 1 - \cos^{2p^2}(\Phi/2)$. For $p = 1$, this Hamiltonian reduces to the interaction of the planar rotator model while for large p, it resembles the Hamiltonian of the n-state Potts model with a n proportional to p. Their conclusion was that this model exhibits BKT transition for small values of p and first order phase transition for relatively large values of p ($p^2 > 10$). This change in the nature of the phase transition for large p may be associated with a large number of vortices that arises almost instantaneously at the transition point [5]. It is in agreement with Minnhagen's proposal [6,7] that in the limit of high particle densities the 2D Coulomb gas model, which is the dual to the planar rotator, would undergo a first order transition. On the other hand, some studies, mostly based on renormalization group analysis, have contested the first order transition [8,9] predicted in the generalized model of references [4,5]. However, a recent rigorous proof [10] has shown that various $SO(n)$-invariant n-vector models with interactions which have a deep and narrow enough minimum have a first-order transition in the temperature. A possibility of the disorder-induced first order transition in the planar rotator model ($V(\Phi) = J_{ij}\cos(\phi_i - \phi_j)$) was also demonstrated by some calculations [11,12], including the discretized Migdal-Kadanoff renormalization group approach [12].

Another model described by the Hamiltonian $H = -J\sum_{i,j}(S_i^x S_j^x + S_i^y S_j^y)$ is the XY-model. The difference in relation to the planar rotator is the number of spin components; in the XY-model the classical spin vector $\vec{S}_i$ is given by (S_i^x, S_i^y, S_i^z), being, therefore, parametrized by two scalar fields, the azimuthal (ϕ_i) and polar (θ_i) angles $\vec{S}_i = (\sin\theta_i\cos\phi_i, \sin\theta_i\sin\phi_i, \cos\theta_i)$. In the sense discussed above, it should also be interesting to study generalizations of this system. Recently, Romano and Zagrebnov [13] have proposed a generalized XY-model defined as follow [13–15]

$$H_{XY}^{Gen} = -J\sum_{\langle i,j\rangle}(\sin\theta_i\sin\theta_j)^q\cos(\phi_i - \phi_j), \tag{1}$$

where $q \in \mathbb{N}$ is the generalization parameter. Note that the emphasis of the generalization is on the variables θ_i and not on Φ as in the planar rotator. Of course, this Hamiltonian has a more complicated dependence on the

[a] e-mail: apereira@ufv.br
[b] *Permanent address*: Institute of Solid State Physics, 72 Tzarigradsko Chaussée, 1784 Sofia, Bulgaria.

spin components as one can see below

$$H_{XY}^{Gen} = -J \sum_{\langle i,j \rangle} [1 - (S_i^z)^2 - (S_j^z)^2 + (S_i^z S_j^z)^2]^{(q-1)/2} \left(S_i^x S_j^x + S_i^y S_j^y\right). \quad (2)$$

For $q = 1$, Hamiltonian (1) recovers the well known XY-model. Our interest is, therefore, in the cases with $q > 1$.

Recent analytical calculations [14] considering the Hamiltonian (1) and based on the continuum theory show that out-of-plane vortex structures (in which the out-of-plane region is restricted to a small core region at the vortex center) are unstable and then, only planar vortex excitations are present. It is in agreement with the usual XY-model. Another result of the continuum approach indicates that the magnon density decreases as $\exp(-\sqrt{q})$, but the planar vortex energy should not be affected. However, as shown by Curie et al. [16], the interaction between soliton structures and magnons provides the sharing mechanism of energy and degrees of freedom among the nonlinear excitations of the system and therefore, it may exist the possibility that, as magnon density decreases, the vortex density should increase. In this respect, it is expected that the vortex density may increase as q increases. Besides, analytical calculations based on some approximated methods such as Mean Field [13] (MF), Two-Site Clusters [13,15] (TSC) and Self Consistent Harmonic Approximation [14] (SCHA), indicate that the critical temperature decreases as q increases. This is another indication that the vortex density should also depend on q. Here we use classical Monte Carlo algorithms to estimate static thermodynamic quantities as a function of the exponent q for several values of temperature T, with emphasis on the internal energy $e = \langle H \rangle / N$, specific heat $c = (\langle H^2 \rangle - \langle H \rangle^2)/(Nk_BT^2)$, magnetic susceptibility of the in-plane spin components, $\chi = (\chi^{xx} + \chi^{yy})/2$, where $\chi^{\alpha\alpha} = \langle (\sum_i S_i^\alpha)^2 \rangle / N$, as well as the vortex densities (N is the number of spins). The critical temperatures obtained here are compared with analytical calculations of reference [14]. Our motivations for the present work are, then, twofold: first, to study the static vortex behavior in more complicated spin systems and check the validity of the approximations used for getting analytical calculations of references [13,14]. Second, to check the possibility of changing the nature of the phase transition (BKT to first order) as the parameter of generalization q increases.

2 Monte Carlo method

We have used a hybrid Monte Carlo approach which includes cluster and single spin updates to calculate some thermodynamic quantities for the model Hamiltonian defined by equation (2). Each Monte Carlo Step (MCS) in our scheme consists of one Wolff [17,18] update of planar components of the spin followed by four Metropolis [19] updates of all the three components and ten overrelaxation steps which changes the configuration but keep the same energy [20,21]. This hybrid algorithm was used to prevent critical slowing down and correlations between different configurations [21–25]. The simulations were performed considering square lattices with periodic boundary conditions (using mostly the lattice sizes $L = 16, 32, 48, 64, 80, 96$). Fixing the generalization parameter q we start with a completely random configuration in the lowest temperature and then 5000 MCS were used for equilibration at each temperature and 100 000 MCS were used to get thermal averages. After the averages are obtained for one temperature, the last configuration is used as the initial one for the next. We also did some simulations varying the generalization parameter q for a given temperature T using the same procedure described above. Most of the results presented here are for lattice size $L = 96$, and other sizes were mainly used to check for significant lattice-size dependence associated with the results. In the figures, the error bars are not shown when the statistical errors are smaller than the symbols. In our notation, the symbol T_{BKT} will be used only for the usual XY-model, i.e., for the case with $q = 1$.

3 Vortex density

Since the thermodynamic quantities have a fundamental dependence on the topological excitations, our first task is to investigate if the exponent q causes changes on the vortex density. Such quantity was obtained based on the work of reference [26]. It is calculated as the thermodynamic average of the absolute value of the vorticity summed over the lattice. Indeed, on going around each plaquette in the lattice, the difference in the angle ϕ of adjacent spins is summed. When this sum is equal 2π (more precisely close to 2π, taking into account possible numerical errors) there is a vortex in this plaquette and if it is -2π there is an antivortex. We have considered only vortices (antivortices) with topological charge $Q = 1$ ($Q = -1$), since they are energetically favorable. Figure 1 shows the vortex (antivortex) density ρ_v as a function of the parameter q for temperature $T = 0.90J$, which is above the critical temperature of the usual XY-model (for $q = 1$, $T_{BKT} = 0.699J$, see Refs. [21,27]) for some lattice sizes. Note that the vortex density increases considerably as q increases. In general, for temperatures above the critical temperature T_{BKT}, the data are well fitted [28] by the following expression

$$\rho_v(T) \approx \rho_0 - \alpha(T) \exp(-\sqrt{q}), \quad (3)$$

where we have used the lattice spacing $a = 1$. The values of ρ_0 and $\alpha(T)$ for several lattice sizes are shown in Table 1. There is no appreciable system-size dependence on the expression and the numerical pre-factor in the exponential term before $\sqrt{q}$ is approximately 1 for all sizes. Expression (3) takes in consideration both vortices and antivortices. The density increases monotonously up to the maximum value $\rho_v^{max} \approx 0.32$, which is independent of the temperature, achieved in the limit $q \to \infty$. A simple argument [29] shows that the maximum vortex density possible in the

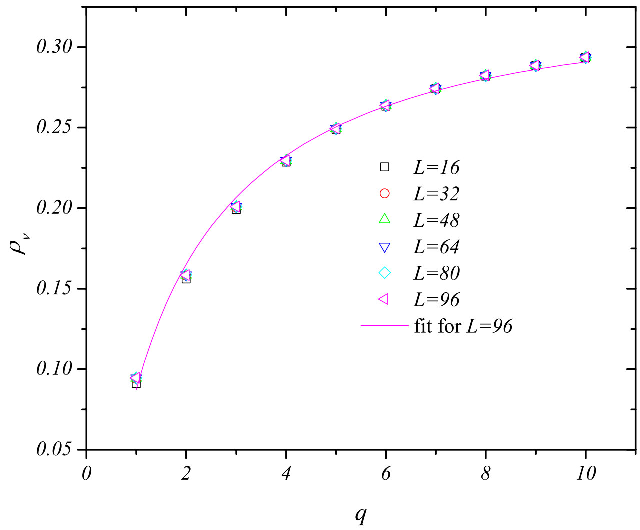

Fig. 1. Vortex density as a function of the exponent q for $T = 0.90$ J and several values of L. The curve is given by equation (4) and correspond to the fit for $L = 96$ with the values given in Table 1.

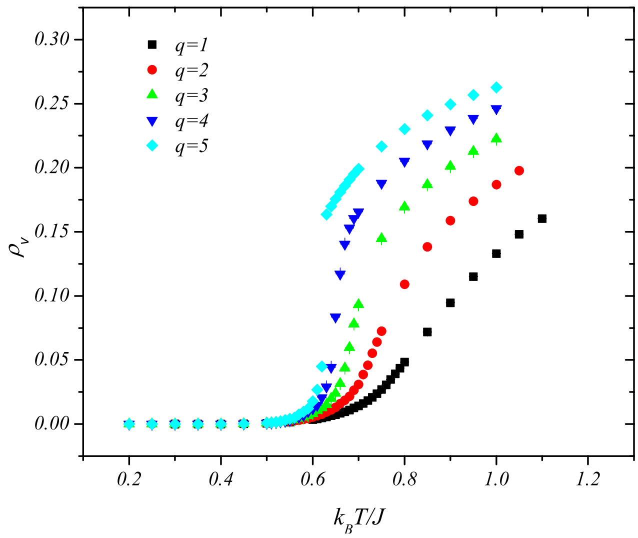

Fig. 2. Vortex density ρ_v versus $k_B T/J$ for $L = 96$. Note that the number of vortices increases considerably for sufficiently large values of q, even for relatively small temperatures.

Table 1. Size dependence of the parameters ρ_0 and $\alpha(T)$. The errors are due to fit uncertainties.

L	ρ_0	$\alpha(T)$
16	0.31768 ± 0.00247	0.63589 ± 0.01485
32	0.31724 ± 0.00244	0.62641 ± 0.01472
48	0.31723 ± 0.00242	0.6253 ± 0.01459
64	0.31726 ± 0.0024	0.62499 ± 0.01443
80	0.31724 ± 0.0024	0.62477 ± 0.01446
96	0.3173 ± 0.00242	0.62545 ± 0.01457

square lattice is 1/6 and hence the saturation density of vortices and antivortices is $1/3 = 0.333$, which is very close to our result for ρ_v^{max}. For the conventional 2D XY-model, this value is achieved in the high-temperature limit ($T \to \infty$). Here, it is achieved in the limit $q \to \infty$, valid for any finite temperature above the critical one, indicating that the parameter q is, to some extent, similar to thermal disorder. In fact, as q increases, vortex density also increases while magnons tend to be suppressed (the correlation length decreases and the magnon density decreases as [14] $\exp(-\sqrt{q})$). Hence, it is reasonable to expect that the critical temperature must also decrease. This can have a simple explanation: above the critical temperature, the correlation length $\xi(T)$ must be interpreted as half of the mean separation between vortices, i.e., $\rho_v \simeq (2\xi)^{-2}$. Since ρ_v increases with q, magnon excitations should become unfavorable as the vortex density (or q) increases. Note that the factor $\exp(-\sqrt{q})$ is present in both vortex and magnon densities, increasing the first and decreasing the second. In the limit $q \to \infty$, the system may contain only vortex excitations. It means that in the high-q limit, the system must be disordered even at very small temperatures, and as a consequence, the critical temperature must be very low. We also plotted the vortex density versus temperature for several values of q in Figure 2. Note that, while for the usual model ($q = 1$) the vortex density increases only gradually with temperature, this density appears to exhibit a sharp jump at a temperature $T(q)$, mainly for $q \gg 1$. Then, for q sufficiently large, vortices suddenly appear in great numbers at some temperature $T(q)$ and following Minnhagen [6,7], Domany et al. [4] and Van Himbergen [5], it may be an indicative that a first order transition takes place. Indeed, the fugacities of the vortices increase until the vortex pairs start overlapping at low enough temperatures when they are supposed to be tightly bound. In fact, it was shown both by analytical calculations (with the help of the generalization of the Kosterlitz renormalization equations [6,7]) and Monte Carlo simulation [30] that this also causes the transition to become first order. As elucidated by Korshunov [11], the Minnhagen criterion for the occurrence of first order transitions in the generalized planar rotator models means that $[\partial^2 V(\cos(\Phi))/\partial\Phi^2]\,|_{\Phi=0}\, /[V(\cos(\pi) - V(\cos(0))] \gg 1$. However, the models considered here also supports a high vortex density at a temperature $T(q)$ and do not obey the Korshunov relation. Our next step is to calculate other thermodynamic quantities as well as the critical temperature $T_c(q)$.

4 Influence of q on the critical temperature and other thermodynamic quantities

Now we consider the effects that the exponent q causes on the critical temperature T_c, the energy e and specific heat c. Firstly, we would like to mention that our results for T_c were obtained considering the same techniques used for the conventional 2D XY-model (i.e., considering a BKT-like phase transition).

Table 2. Critical temperature estimated by the methods described in the text. The errors correspond to statistical deviations.

q	Binder's cumulant	η	Υ	FSS of Υ	SCHA
2	0.687 ± 0.003	0.665 ± 0.003	0.662 ± 0.001	0.653 ± 0.002	0.848
3	0.656 ± 0.003	0.637 ± 0.001	0.632 ± 0.002	0.624 ± 0.003	0.700
4	0.631 ± 0.002	0.615 ± 0.002	0.613 ± 0.001	0.604 ± 0.001	0,595
5	0.609 ± 0.006	0.599 ± 0.001	0.598 ± 0.001	0.592 ± 0.002	0.518

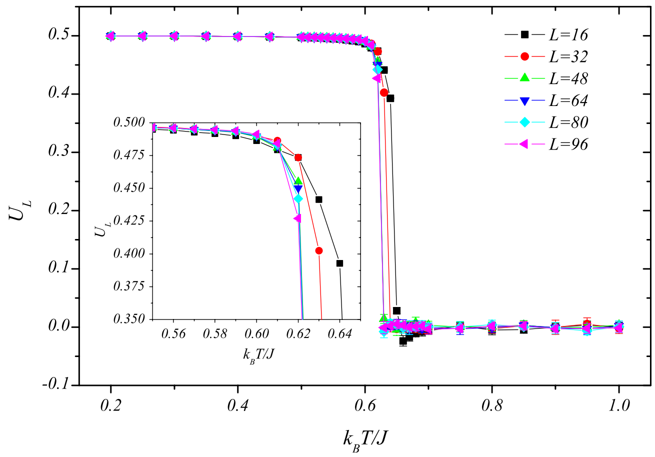

Fig. 3. Cumulant of magnetization for $q = 5$ for several lattice sizes. The inset show the crossing region in more details.

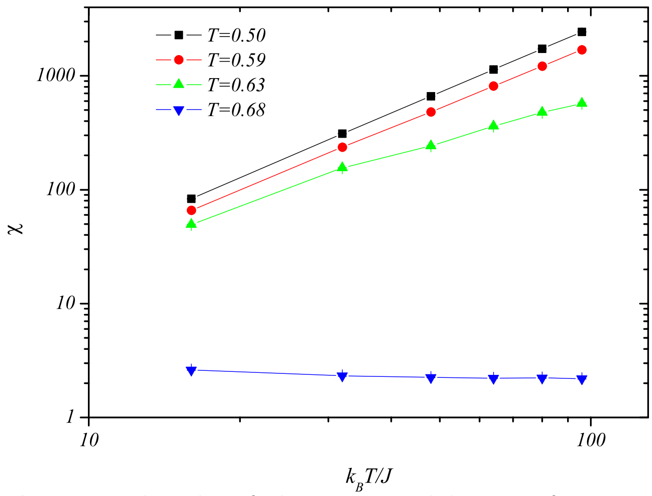

Fig. 4. Log-log plot of planar susceptibility as a function of the lattice sizes for $q = 5$ and some values of temperature. The slope of the curves is $2 - \eta$.

4.1 Influence on critical temperature

To locate the critical temperature we apply three different methods usually considered for Berezinskii-Kosterlitz-Thouless (BKT) like phase transitions, namely the size dependence of Binder´s fourth order cumulant, susceptibility exponent η and helicity modulus Υ. The numerical values of T_c obtained by these methods for some values of q are summarized in Table 1. They are also compared to the SCHA method [14,31,32].

4.1.1 Binder´s fourth order cumulant

A rough estimative of T_c could be obtained by using the size-dependence of Binder's fourth order cumulant [33,34, 23,24] U_L, defined as follows

$$U_L = 1 - \frac{\langle (M_x^2 + M_y^2)^2 \rangle}{2\langle M_x^2 + M_y^2 \rangle^2}, \quad (4)$$

where M_x and M_y are the in-plane magnetization components. For any lattice size L, the asymptotic values are $U_L(T \ll T_c) = 0.5$, $U_L(T \gg T_c) = 0$. At the critical temperature, U_L is approximately independent of L, hence, T_c can be estimated from the crossing point of curves of U_L for several L. However, for large values of q the curves start to overlap in a large temperature range, which makes the estimative of the critical temperature by this method very imprecise, as can be seen in Figure 3 (for $q = 5$). The results for the critical temperature obtained by this method are given in Table 2.

4.1.2 Susceptibility exponent η

Another method that could be used to estimate the critical temperature for BKT-like phase transitions is the finite-size scaling of the planar susceptibility as was used by Cuccoli et al. [27] and Wysin and co-workers [23,24]. It is expected for the XY and PR models that the in-plane magnetic susceptibility (χ) has a power law behavior near and below the critical temperature according to

$$\chi \propto L^{2-\eta}, \quad (5)$$

were η is the exponent for the in-plane spin correlations below T_c (for details see Ref. [27]). We can calculate the exponent η, as a function of temperature, by fitting [28] the susceptibility for several lattice sizes to the above expression for each temperature. For XY and PR models T_c is estimated when $\eta = 1/4$. Here we assume that even for the generalized XY models (with $q \neq 1$) the exponent η is equal to $1/4$ at critical temperature, and that this power law behavior still holds. In Figure 4 we show the log-log plot of the susceptibility versus L for $q = 5$ and several temperatures. The slope of the curves is $2-\eta$. In Figure 5 (also for $q = 5$) the exponent η, obtained by fitting the data to equation (5), is shown as a function of the temperature. The results for the critical temperature obtained by this method are given in Table 2.

4.1.3 Helicity modulus Υ

The helicity modulus is a measure of the resistance to an infinitesimal spin twist Δ across the system along one

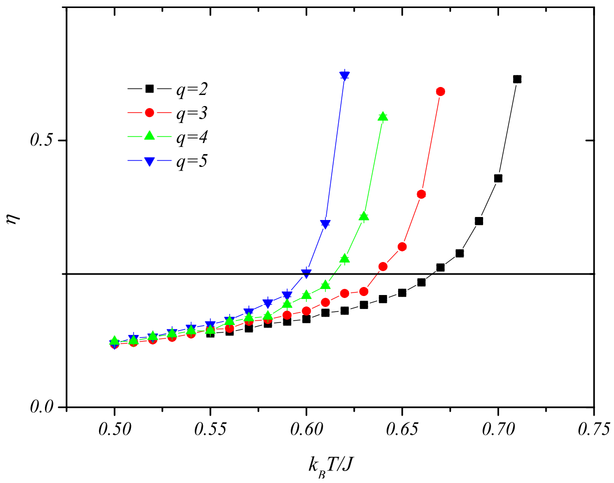

Fig. 5. Temperature dependence of η. The critical temperature is estimated when $\eta = 1/4$.

coordinate, expressed in terms of the dimensionless free energy, $f = F/J$,

$$\Upsilon(T) = \frac{1}{N}\frac{\partial^2 f}{\partial \Delta^2}. \tag{6}$$

For the generalized XY-model, defined by equation (1), one could show that

$$\Upsilon(T) = \frac{1}{2}\langle H\rangle - \frac{1}{Nk_BT}\left\langle \left[J\sum_{\langle i,j\rangle}(\sin\theta_i \sin\theta_j)^q \cos(\phi_i - \phi_j)\hat{e}_{ij}\cdot\hat{x}\right]^2\right\rangle, \tag{7}$$

where $\langle H\rangle = \langle H_{XY}^{Gen}\rangle/N$ is the energy per spin (e) and $\hat{e}_{ij}$ is a unit vector pointing from site i to site j. According to renormalization-group theory, the helicity modulus in an infinite system jumps from the finite value $(2/\pi)k_BT_c$ to zero at the critical temperature. Therefore, an estimative of the critical temperature could be obtained simply by locating the intersection of Υ as a function of T and the straight line

$$\Upsilon = \frac{2}{\pi}k_BT, \tag{8}$$

as shown in Figure 6. Better results are obtained by applying finite-size scaling analysis. An useful scaling expression is [23,35–37],

$$\frac{\pi\Upsilon}{2k_BT} = A(T)\left[1 + \frac{1}{2\ln(L/L_0)}\right], \tag{9}$$

with $A(T)$ and L_0 being fitting[28] constants. This expression is exact at $T = T_c$, with $A(T_c) = 1$ (see Ref. [23] and references therein). So, we can find T_c by locating the temperature where $A(T) = 1$. The function $A(T)$ is shown in Figure 7. The results obtained are also shown in Table 2.

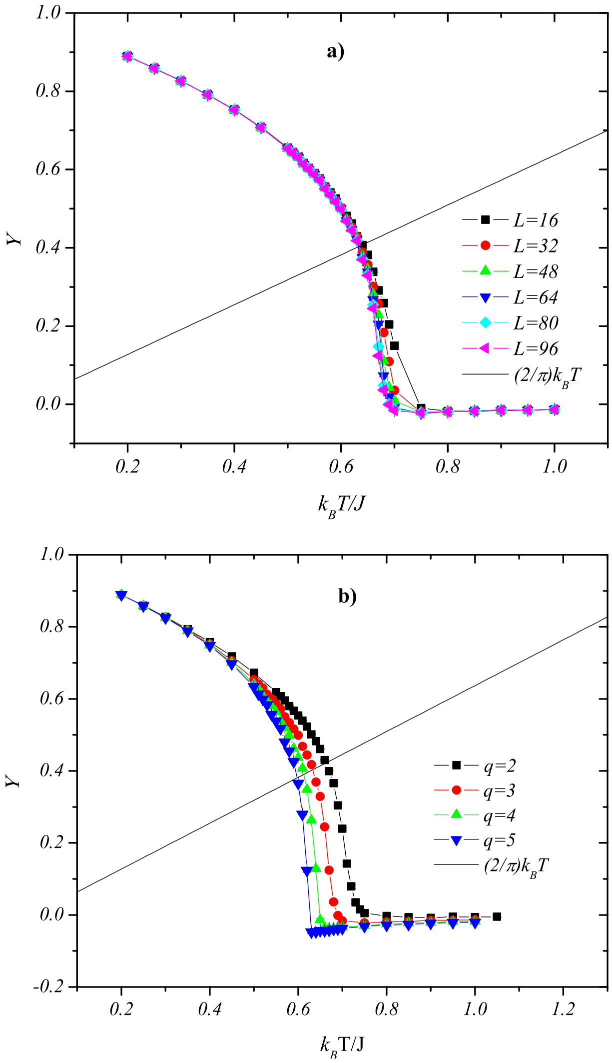

Fig. 6. (a) Helicity modulus as a function of temperature for several lattices sizes for $q = 3$. (b) Helicity modulus as a function of temperature for $L = 96$ and $q = 2, 3, 4$ and 5.

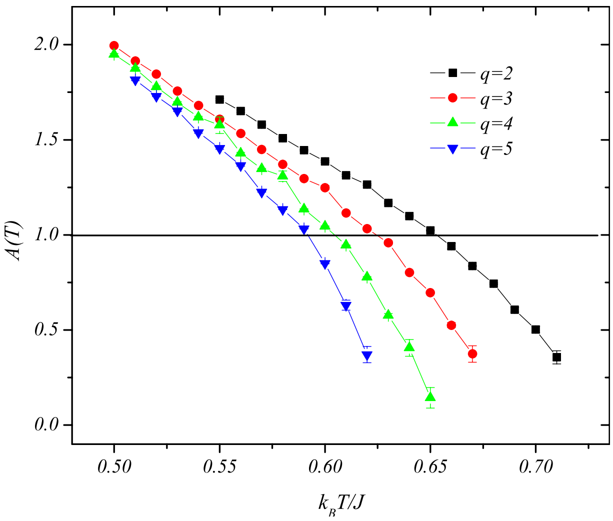

Fig. 7. Fitting parameter $A(T)$ as a function of temperature for some values of q.

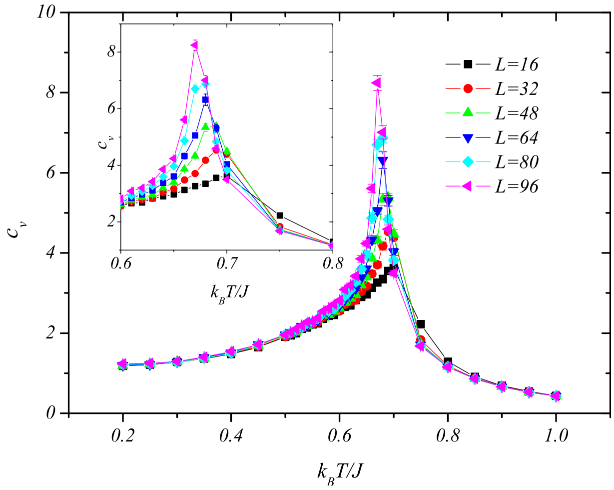

Fig. 8. Specific heat for $q = 3$ and several lattice sizes. Note that finite-size effects are very pronounced.

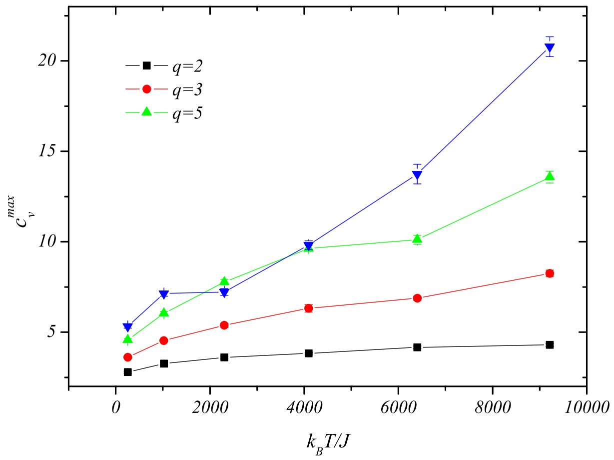

Fig. 9. Specific heat maximum (c_v^{max}) for some values of q versus L^2.

4.2 Energy and specific heat

Figure 8 shows the specific heat for the simulated lattice sizes and $q = 3$. In contrast to what happen in the usual XY model ($q = 1$), where finite-size effects are very small [27], these effects become considerable as q increases. In fact, the specific heat peak moves toward lower temperatures and becomes narrower and higher as L increases. The high values of the specific heat peak indicate the possibility that a first-order phase transition takes place. Really, for this type of phase transition, it is expected that the maximum value of the specific heat (c_v^{max}) has a proportionality relation with the volume of the system [34], i.e., $c_v^{max} \propto L^d$ where d is the system dimension (in our case $d = 2$). In Figure 9, we plotted the specific heat maximum [38] versus L^2 for some values of q. Note that, although the c_v^{max} increases considerably with L, it does not have exactly a linear dependence with L^2. Tests were also made using smaller temperature steps, but the results are very similar. So we can not be conclusive about

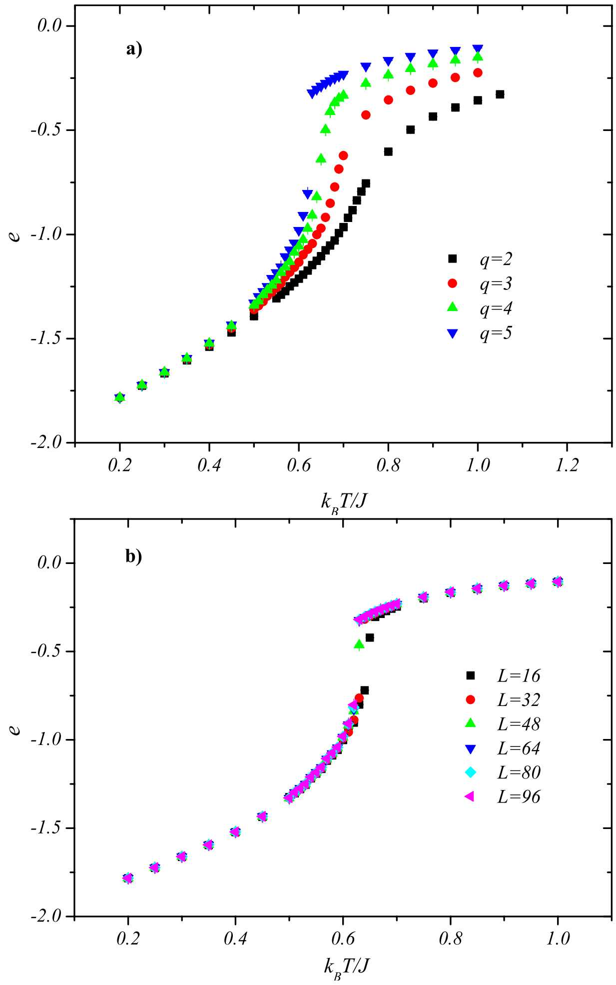

Fig. 10. (a) Energy per spin versus temperature for some values of q and $L = 96$. (b) Energy for $q = 5$ and several lattice sizes.

a possible change of the nature of the phase transition using these considerations. Concerning still the specific heat, we remark that its maximum is located above the critical temperature for the usual XY-model [39] (approximately ten percent above T_{BKT}). This may be qualitatively understood in terms of a sequential unbinding of vortex-antivortex pairs in multiple-bound clusters. However, as q is increased, the difference between the position of the specific heat peak and the critical temperature decreases slowly. Our results show that for $q = 2$ the specific heat maximum (for $L = 96$) is located about 8.7% above the critical temperature (obtained by FSS of the helicity modulus) while for $q = 5$ it is located about 4.7% above T_c.

In Figure 10 the average energy per site e is plotted as a function of T. Again, for sufficiently large values of q, there is a near discontinuity in e exactly at the same point where the specific heat exhibits a large and sharp peak. In fact, this is approximately the same point where the vortex density exhibits a sharp jump.

Again, to check the possibility of a first-order phase transition we also performed simulations increasing temperature and then decreasing, in order to look for

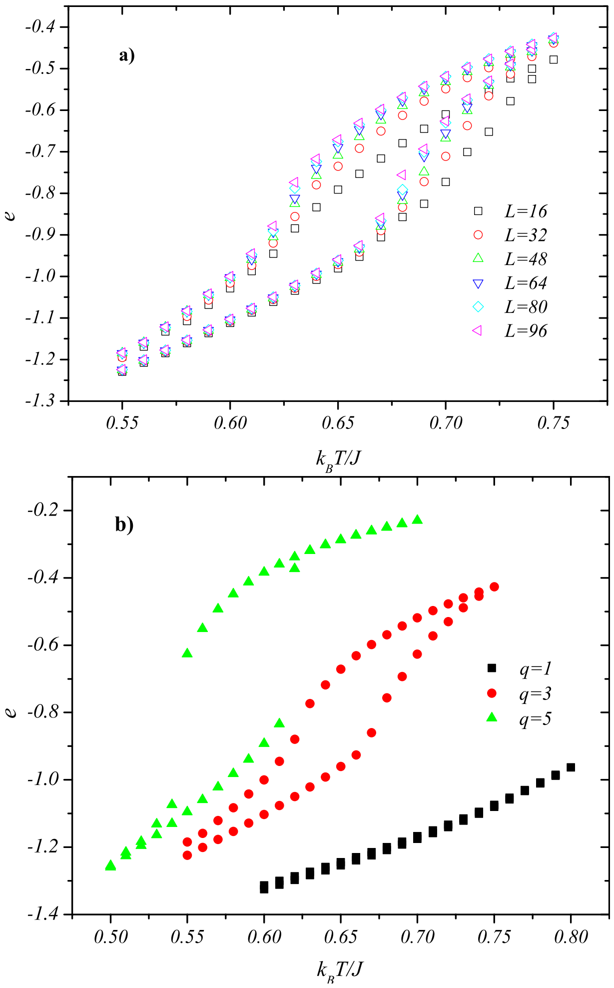

Fig. 11. (a) Size dependence of the hysteresis curve for $q = 3$. Note that hysteresis persist even to the largest lattice size simulated. (b) Hysteresis curves for $q = 1, 3$ and 5 and $L = 96$.

hysteresis effects. In fact, we observe that as q increases hysteresis starts to appear and persists even if the number of MCS used for equilibration (not shown here) or the lattice size (see Fig. 11) are increased. However, the histograms of energy does not exhibit double peak structure. In summary, although our results can not be conclusive, they suggest that the hysteresis observed in the energy (see Fig. 11), the jump in the vortex density, the peak in the specific heat and the discontinuity in the energy, all happening at the same point may be an indicative that the system also exhibits a first order transition [5] for large enough values of q.

5 Discussions

In this work we have performed MC simulations for studying an interesting generalization of the 2D XY-model. The critical temperature $T_c(q)$, the vortex density, internal energy, specific heat and magnetic susceptibility were obtained. The values of T_c were calculated by using three methods based on the BKT transition. We have to say, however, that this study is only a first step in direction to a more elaborated theory. Really, lacking a detailed theory for these generalized XY-models, we had to use expressions and methods available for the standard $2D$ model. However, the high vortex density (see Sect. 3) and the results of Section 4 also suggest that a first order transition at a temperature slightly above $T_c(q)$ calculated here may occur for large enough q. Hence, our results give some support to the idea that the generalized model (1) in two dimensions may undergo two distinct transitions due to the influence of strong disorder (large number of vortices and strong out-of-plane fluctuations for high values of q). It is not conclusive, but if the first order transition really happens, the critical point of this transition should be very near the one calculated using BKT methods, mainly for $q \gg 1$. This small difference may be the cause of the absence of a clear identification of this point in these complicated spin models, which contain three spin components interacting in a nontrivial way. It is possible that vortices alone are sufficient to account for these two kinds of transitions but, of course, in a qualitatively different manner. The BKT transition is based on the vortex-pairs unbinding and the first-order transition, in this case, would be associated with a large number of vortices that appear in the system instantaneously. These two phenomena arise almost at the same temperature. For instance, the case $q = 5$ in Figure 2 shows clearly this process. As the temperature is increased from zero, the vortex pair density starts to grow simultaneously with an increase of the size of the pairs. There is only a few vortices in the temperature range $0 < T < 0.6J$. At $T \approx 0.6J$, vortices start to appear everywhere and the vortex density changes drastically from almost zero to almost saturation ($\rho_v^{max} = 1/3$). After that, the process becomes extremely complicated. As vortices become denser, there is less space to put in new pairs and hence the average pair size decreases for sufficiently high temperature. With many vortices in the lattice, the process of creation and annihilation of pairs may become extremely relevant causing another type of transition. To conclude, we would like to mention that these generalized models may be also useful to give some insights about the static and dynamical behavior of systems containing a high vortex density. For instance, magnetic 2D systems with a percentage of nonmagnetic impurities seem to exhibit this characteristic [23–25].

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