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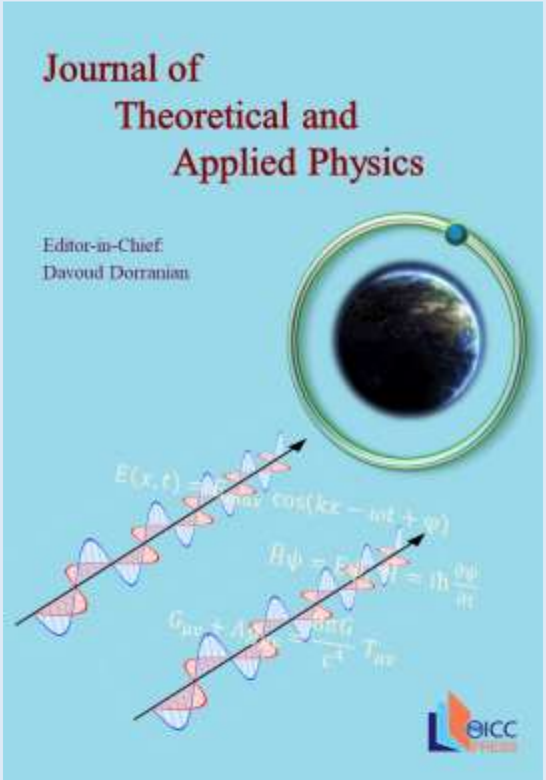

Effect of long-range interactions on the Kosterlitz-Thouless transition

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Abstract

The two-dimensional XY model of continuous spins on a square lattice is studied by Monte Carlo simulations in the nonextensive statistical approach of Tsallis, using the Metropolis algorithm with a transition probability of the nonextensive approach. Energy per spin, magnetization per spin, heat capacity, magnetic susceptibility, Binder cumulant of the magnetization and Binder cumulant of the energy are calculated in a temperature interval between 0.02 and 2 with a step of 0.02, for square lattice sizes considered between 12^2 and 48^2, with periodic boundary conditions, and for discrete values of the Tsallis entropic index q used between 0.99 and 0.5. It has been found that the Kosterlitz-Thouless transition is well observed and modified for $q = 0.99$ and 0.9 ; its critical temperature decreases when q decreases. A particular behavior of the system evolution is observed for $q = 0.8$ and 0.7. The absence of phase transitions was confirmed for $q \leq 0.6$.

Keywords: two-dimensional XY model, Kosterlitz-Thouless transition, Tsallis statistics, Monte Carlo simulation.

1. Introduction

The application of a specific statistical approach to a physical system essentially depends on the nature of the microscopic interactions, the microscopic memory [1][2]. For short-range-interactions and for non-(multi)fractal boundary conditions, the usual Boltzmann-Gibbs statistic is sufficient. However, for systems with dominant long-range-interactions, a more generalized statistical approach will be needed [3]. Black holes and superstrings [4][5], granular matter [6], two-dimensional turbulence [7][8], astrophysics and the many-body-gravitational problem [9][10] are some examples of this type of systems. An important generalization of the Boltzmann-Gibbs statistic was proposed in 1988 by Tsallis [11], called "nonextensive statistic", it is based on a new entropy formula with an index characterizing the influence of long-range-interactions. In recent years, the Tsallis statistic has been successfully applied in different fields [12] such as biology [13][14], chemistry [15] and physics [16][17][18][19].

Monte Carlo simulations are recently performed to study phase transitions in magnetic systems using the Tsallis statistical approach. In most of these studies, discrete spin models are used such as the two-dimensional uniform Ising model [16][20][21], the two-dimensional Potts model [22]. However, models of continuous spins possessing important particular properties are not yet studied by this method.

The objective of this paper is to study a simple classical model of continuous spins, which is the two-dimensional XY model, and its phase transitions by Monte Carlo simulation in the Tsallis statistical approach, using a simple generalization of the Metropolis algorithm. Thermodynamic observables will be calculated and studied over a temperature interval for different values of an entropic index called “Tsallis entropic index”, which depends on the difference between Boltzmann-Gibbs and Tsallis statistics.

2. Two-dimensional XY model and Kosterlitz-Thouless transition

The XY model describes a system of two-dimensional unit spin vectors located at sites of a two-dimensional or three-dimensional lattice, with nearest-neighbor interactions. The spin $\vec{s}_i(s_{i,x} = \cos\theta_i \,, s_{i,y} = \sin\theta_i)$ with $|\vec{s}_i| = 1$ located in site i can rotate in a plane at an angle $\theta_i \in [0\,, 2\pi]$ with respect to a specified direction [23][24]. The Hamiltonian of this model is given by:

$$H = -J\sum_{\langle ij\rangle}\cos(\theta_i - \theta_j) + h\sum_i \cos\theta_i \qquad (1)$$

where J is the spin-spin coupling interaction and h is the external field interaction. The notation $\langle ij\rangle$ means a summation over the nearest neighbor sites only. In this work we take $h = 0$ to eliminate the source term breaking the symmetry. In this case the energy is of O(2) symmetry, that is to say a rotation of all the spins by the same angle, does not change the energy of the system [23].

The two-dimensional XY model is widely used to study the physical and critical behavior of a few two-dimensional systems such as superfluid helium thin films [25], superconducting thin films [26], ferromagnetic layers [27], crystal surfaces [28] and two-dimensional Coulomb gas [29]. Although it can be rigorously proven that the order parameter (the magnetization) of the XY model is zero at any finite temperature in two dimensions, and that the susceptibility is finite at high temperature but diverges at a critical temperature, there is good evidence that the Two-dimensional XY model undergoes a very specific transition of infinite order, known as the "Kosterlitz-Thouless transition" [30][31]. Experimentally, thin films of liquid helium and superconducting materials seem to show this transition. Numerous numerical studies have been carried out to confirm the predictions of this transition and to estimate its critical temperature. Most of them are Monte Carlo studies. Some authors have studied the existence of the classical first-order and second-order phase transitions for the two-dimensional XY model in special cases [32][33]. Kosterlitz and Thouless [30][31] showed that there is another set of excitations that takes the system from its ordered phase at low temperature, well described by the spin wave approximation, to a disordered state at high temperature with exponentially decreasing correlations. These new excitations are identified as topological defects in the form of "vortices" created by the spins. The defects are observed as low-temperature bonded vortex-antivortex pairs. By increasing the temperature, the vortex-antivortex pair detaches at the critical point of the Kosterlitz-Thouless transition. However, no specific thermal anomaly is observed at this point. The energy of an isolated vortex is much higher than that of a pair of closely related vortices. Thus, it takes much less energy for a pair of tightly bound vortices to exist than to unbind to form two isolated vortices. Accordingly, at sufficiently low temperatures where there is not enough thermal energy to unbind the vortex pairs, there exists a state which consists of an equilibrium density of bound vortex pairs. At higher temperatures, the thermal energy becomes more prominent and able to untie the vortex pair. The critical temperature in the Kosterlitz-Thouless transition at which the vortices begin to untie is estimated to be $T_{KT} \simeq 0.8929\, J/k_B$, where J is the spin-spin coupling constant and k_B is the Boltzmann constant.

The absence of long-range order, the presence of topological defects called "vortices", and the Kosterlitz-Thouless transition are some of the important properties of the two-dimensional XY model for which it is markedly different from other two-dimensional classical systems.

3. Tsallis statistical approach

In order to include long-range-interactions in the statistical description of complex systems, a generalization of the usual Boltzmann-Gibbs statistics was proposed by Tsallis in 1988 [11], which is based on the following entropy formula:

$$S_q = k_B \frac{1 - \sum_{i=1}^{\Omega} p_i^q}{q - 1} \tag{2}$$

where k_B is the Bolzmann constant, Ω is the number of possible microstates of the system, q is a real parameter characterizes the degree of the deformation of the statistics or of the nonextensivity, called "Tsallis entropic index" and p_i $(0 < p_i < 1)$ is the probability that the system is in microstate i such that $p_i < p_i^q$ for $q > 1$ and $p_i > p_i^q$ for $q < 1$. When $q = 1$ the usual Boltzmann–Gibbs statistic will be found. For this reason we have chosen discrete values of $q \leq 1$ in this paper. Note that in Monte Carlo simulations we cannot take continuous values of q.

The most important property of the Tsallis entropy is its nonextensive nature. Indeed, for a system consisting of two subsystems A_1 and A_2, then the Tsallis entropy of the global system is:

$$S_q(A_1 + A_2) = S_q(A_1) + S_q(A_2) + \frac{1 - q}{k_B} S_q(A_1) S_q(A_2) \tag{3}$$

For $q = 1$ the entropy S_q therefore becomes extensive.

In nonextensive statistics, the q-mean value of a thermodynamic observable X is given by:

$$\langle X \rangle_q = \sum_i p_i X_i \tag{4}$$

where p_i are the escort probabilities defined by:

$$p_i = \frac{p_i^q}{\sum_i p_i^q} \tag{5}$$

the q-average value of the generalized internal energy U_q is defined as:

$$U_q = \langle H \rangle_q = \sum_i p_i E_i \tag{6}$$

where H is the Hamiltonian of the system and E_i is the energy of possible state i.

the canonical distribution adapted to Monte Carlo simulations [22] is given by:

$$p_i = \frac{1}{Z_q} [1 - (1 - q)\beta' E_i]^{\frac{1}{1-q}} \tag{7}$$

with

$$\beta' = \frac{\beta}{\sum_i p_i^q + (1 - q)\beta U_q} \tag{8}$$

$$\beta = \frac{1}{k_B T} \tag{9}$$

$$Z_q = \sum_{i=1}^{\Omega} [1 - (1-q)\beta' E_i]^{\frac{1}{1-q}} \tag{10}$$

where β' is the Lagrange multiplier associated with the energy constraint, k_B is the Boltzmann constant, T is the thermostat temperature and Z_q is the generalized canonical partition function. The choice of temperature in the Tsallis statistic poses a problem during the simulation. In this work, we have chosen $1/\beta'$ as the temperature scale, as they did the authors of references [16][22].

4. Metropolis algorithm in the Tsallis statistical approach

The implementation of the XY model using the simple Metropolis [34] Monte Carlo algorithm in the non-extensive statistics approach is done by the following steps:

1) Choose a random initial configuration of the studied spin lattice.
2) Randomly change the orientation of each spin in the lattice.
3) Calculate the difference ΔE in energy due to the change in spin orientation using the Hamiltonian of the XY model.
   - If $\Delta E \leq 0$ keep the new spin orientation.
   - If $\Delta E > 0$ generate a random number $r \in [0\,,1]$, and calculate the probability p of transition in the nonextensive statistic:

$$p = \left[\frac{1-(1-q)\beta' E_j}{1-(1-q)\beta' E_i}\right]^{1-q} \tag{11}$$

   If $r \leq p$ keep the new spin orientation.
4) Repeat N_{eq} times the steps 2 and 3 until thermal equilibrium is reached. N_{eq} is the number of Monte Carlo steps needed to reach thermal equilibrium.
5) Calculate the statistical q-mean on the possible configurations of the thermodynamic quantities X and on a number of Monte Carlo steps $N - N_{eq}$ with $N > N_{eq}$, i.e.:

$$\langle\langle X\rangle_q\rangle_{MC} = \frac{1}{(N - N_{eq})} \sum_{i=N_{eq}}^{N} \langle X\rangle_{q,i} \tag{12}$$

where $\langle\ldots\rangle_q$ means the statistical q-mean over the possible configurations and $\langle\ldots\rangle_{MC}$ means the mean over a number $N - N_{eq}$ of Monte Carlo steps.

In this generalized Metropolis algorithm, the transition probability of the Boltzmann-Gibbs statistic has been replaced by that of the Tsallis statistic as the case of the references [16][22].

5. Simulation results

Monte Carlo simulations using the Metropolis algorithm [34] in the Tsallis statistical approach are performed on a square lattice of $N = L^2$ spins, which is described by the two-dimensional XY model. Periodic boundary conditions have been applied to edge spins. The quantities calculated are:

the energy per spin:

$$e(L,T,q) = \langle\langle \frac{1}{N}\sum_{l=1}^{N}\left(-J\sum_{\langle ij\rangle}\cos\left(\theta_{i,l}-\theta_{j,l}\right)\right)\rangle_q\rangle_{MC} \tag{13}$$

the magnetization per spin:

$$m(L,T,q) = \langle\langle \frac{1}{N}\sqrt{\left(\sum_{i=1}^{N}\cos\theta_i\right)^2 + \left(\sum_{i=1}^{N}\sin\theta_i\right)^2}\rangle_q\rangle_{MC} \tag{14}$$

the magnetic susceptibility:

$$\chi(L,T,q) = \frac{1}{k_B T}\left(\langle\langle m^2\rangle_q\rangle_{MC} - \langle\langle m\rangle_q{}^2\rangle_{MC}\right) \tag{15}$$

the heat capacity:

$$C_V(L,T,q) = \frac{1}{k_B T^2}\left(\langle\langle e^2\rangle_q\rangle_{MC} - \langle\langle e\rangle_q{}^2\rangle_{MC}\right) \tag{16}$$

the Binder cumulant of the magnetization:

$$U_m(L,T,q) = 1 - \frac{\langle\langle m^4\rangle_q\rangle_{MC}}{3\langle\langle m^2\rangle_q{}^2\rangle_{MC}} \tag{17}$$

and the Binder cumulant of the energy:

$$U_e(L,T,q) = 1 - \frac{\langle\langle e^4\rangle_q\rangle_{MC}}{3\langle\langle e^2\rangle_q{}^2\rangle_{MC}} \tag{18}$$

To simplify, we have taken the coupling constants $J = 1$ and the Boltzmann constant $k_B = 1$, in this case the temperature and the calculated quantities are given in reduced units. Square lattice sizes are chosen between 12^2 and 48^2. A temperature interval is chosen between 0.02 and 2 with a step of 0.02. A total number of Monte Carlo steps $N = 6 \cdot 10^4$ is used, of which $N_{eq} = 10^4$ is associated to reach thermal equilibrium. The calculations are made in the case of the extensive Boltzmann-Gibbs statistic and in the case of the nonextensive Tsallis statistic for values of the Tsallis entropic index q between 0.99 and 0.5.

Figure 1 shows the curves of variation of ; energy per spin e, magnetization per spin m, heat capacity C_V and magnetic susceptibility χ as a function of temperature, for a square lattice size

$L^2 = 48^2$ with different values of the entropic index q and for the case of the Boltzmann–Gibbs statistic. It can be seen that the Kosterlitz-Thouless transition is well observed for $q = 0.99$ and 0.9. Specific behaviors are observed for $q = 0.8$ and 0.7; the curves of m (resp. the curves of e) have a maximum (resp. a minimum) then an inflection, this is valid whatever the size of the lattice square as shown in **figure 2**. The magnetization and the energy per spin strongly depend on q at low temperatures, i.e. in the first phase of transition. Indeed, when q decreases m decreases and e increases. The heat capacity curves have a maximum which moves to the left when q decreases, the maximum disappears for $q < 0.8$. The same remark was observed for the susceptibility curves, except that the maximums only disappear for $q < 0.5$. However, for $q = 0.8$ there are two maxima, this is remarkable whatever the lattice size as shown in **figure 2**. Moreover, when the size of the system increases the peaks of the maximums become sharper. We also notice that the critical temperature corresponds to the maximum of the heat capacity decreases when q increases. For $q \leq 6$ the system have no phase transition. For $q = 0.99$ the results obtained are very close to those obtained in the case of the extensive Boltzmann-Gibbs statistics.

To estimate the critical temperature of the studied transition at the thermodynamic limit ($L \longrightarrow \infty$), we plotted the Binder cumulant of the magnetization as a function of temperature for $L^2 = 48^2$, for different values of q and for the case of the Boltzmann–Gibbs statistic on one side (see **figure 3 (a)**), and for $q = 0.9$ with different values of L on the other side (see **figure 3 (b)**). From **figure 3 (a)** it was again found that the critical temperature T_C strongly depends on q, and for $q = 0.7$ and 0.8 a specific behavior is observed. The point of intersection of the curves of **figure 3 (b)** corresponds to T_C at the thermodynamic limit for $q = 0.9$. Estimated values of T_C by this method for different values of q are given in **table 1**. It has been found that T_C decreases as q decreases at the thermodynamic limit. Note that to obtain a value of T_C close to that of the Kosterlitz-Thouless transition $T_{KT} \simeq 0.8929\, J/k_B$ by performing simulations in the case of the Boltzmann-Gibbs statistics, it is necessary to choose large values of L, this requires a machine powerful.

Another method is often used to estimate T_C at the thermodynamic limit, which consists of the linear fitting of the curves of T_C according to $(1/L^2)$; the ordinate at the origin of the line obtained by linear fitting is the critical temperature at the thermodynamic limit. **Figure 4** shows an example for $q = 0.9$ using the values of T_C corresponding to the maximum of the heat capacity curves. The results obtained by this method are also given in **table 1**.

In order to compare the Kosterlitz-Thouless transition with classical transitions, we plotted the Binder cumulant of the energy U_e as a function of the temperature; for $L^2 = 48^2$ with different values of q and the case of the Boltzmann–Gibbs statistic on one side (see **figure 5 (a)**), and for $q = 0.9$ with different values of L on another side (see **figure 5 (b)**). It has been found that for the Kosterlitz-Thouless transition there is no minimum on the Binder cumulant of energy curves unlike the case of classical transitions. Moreover, the appearance of this transition on the curves of U_e strongly depends on L and q.

6. Conclusions

A study by Monte Carlo simulations is carried out in the nonextensive statistical approach of Tsallis, applied to the XY model on a square lattice of continuous spins, with nearest neighbor interactions and periodic boundary conditions. It is based on a simple generalization of the Metropolis algorithm by replacing the transition probability of the extensive Boltzmann-Gibbs statistic by that of the nonextensive Tsallis statistic. The average values of energy per spin, magnetization per spin, heat capacity, magnetic susceptibility, Binder cumulant of magnetization and Binder cumulant of energy are calculated in an interval of temperature $0.02 \leq T \leq 2$ with a step of 0.02. Square lattice sizes are chosen between 12^2 and 48^2 with discrete values of the Tsallis entropy index q between 0.99 and 0.5 are used. The results obtained in the nonextensive statistical approach when $q \longrightarrow 1$ tend towards those obtained in the extensive statistical approach. The Kosterlitz-Thoules transition characterizing the two-dimensional XY model has been well observed and modified for $q = 0.99$ and 0.9. Its critical temperature T_C estimated in the thermodynamic limit is proportional to q. A particular behavior of evolution of the system was observed for $q = 0.8$ and 0.7. For $q \leq 6$ there is no observed transition. The Binder cumulant of energy does not have a minimum in the case of the Kosterlitz-Thoules transition. When applying the two-dimensional XY model, consideration must be given to long-range-interactions.

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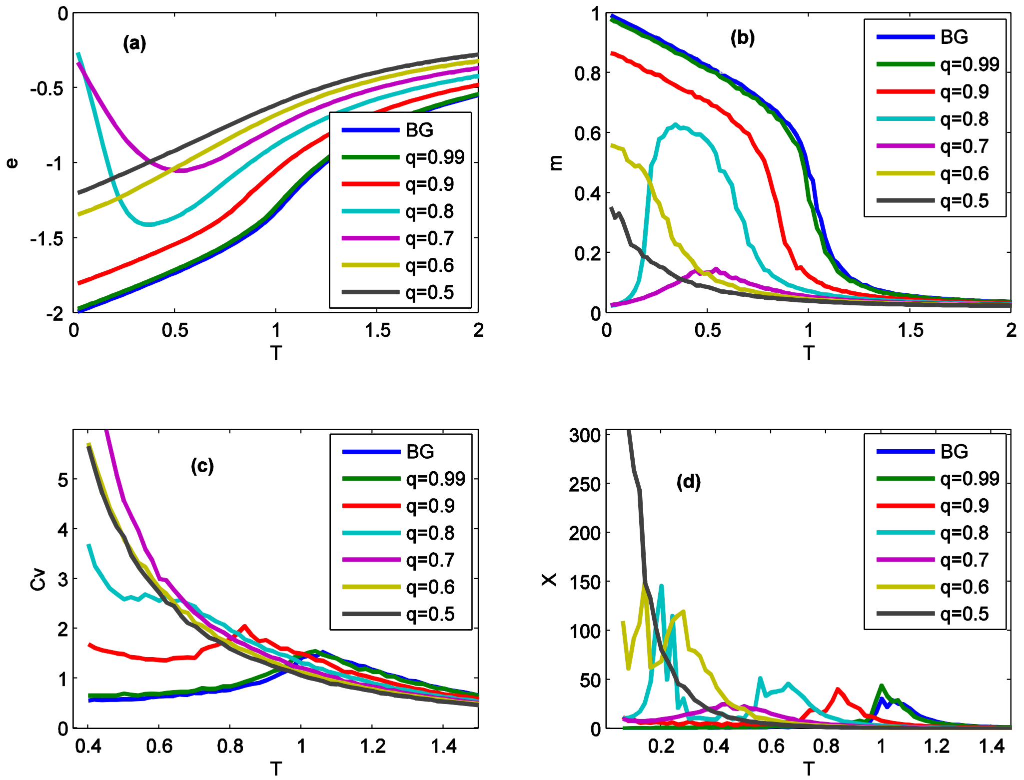

Figure 1 : Curves of variation of: **(a)** energy per spin, **(b)** magnetization per spin, **(c)** heat capacity, **(d)** magnetic susceptibility; as a function of temperature, in the case of the XY model on a square lattice of size $L^2 = 48^2$, for different values of the Tsallis entropic index q. BG means the Boltzmann-Gibbs statistic.

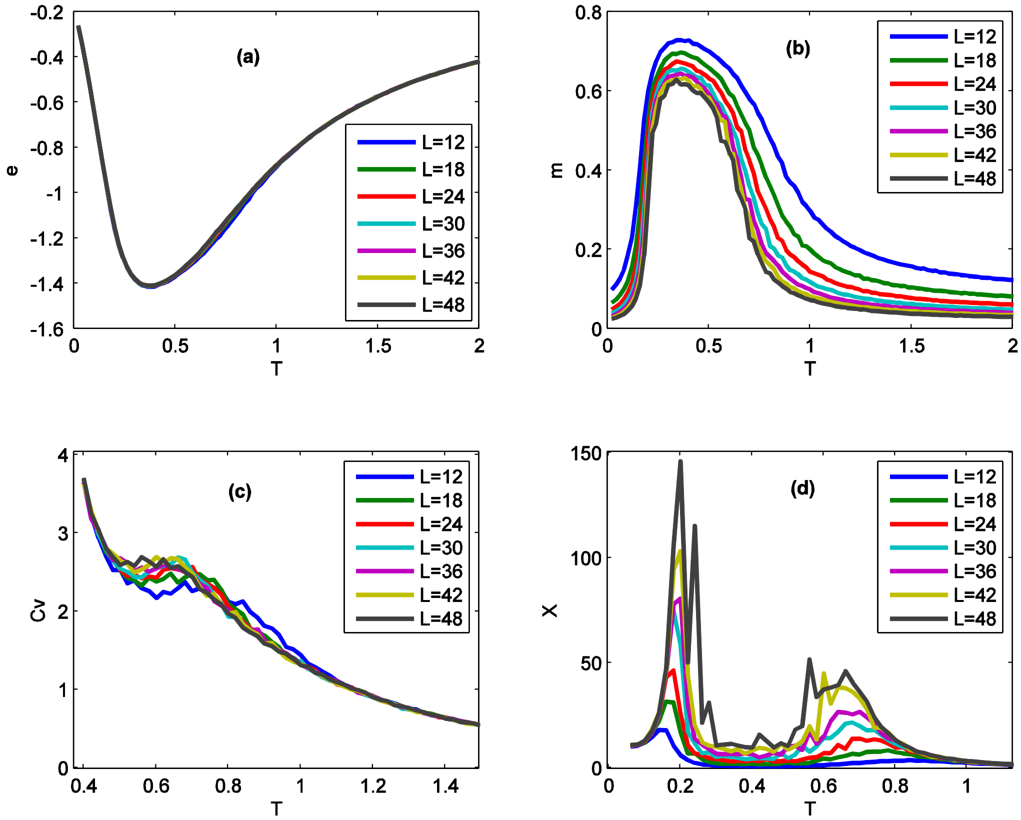

Figure 2 : Curves of variation of: **(a)** energy per spin, **(b)** magnetization per spin, **(c)** heat capacity, **(d)** magnetic susceptibility; as a function of temperature, in the case of the XY model on a square lattice at different sizes L^2, for the value of the Tsallis entropic index $q = 0.8$.

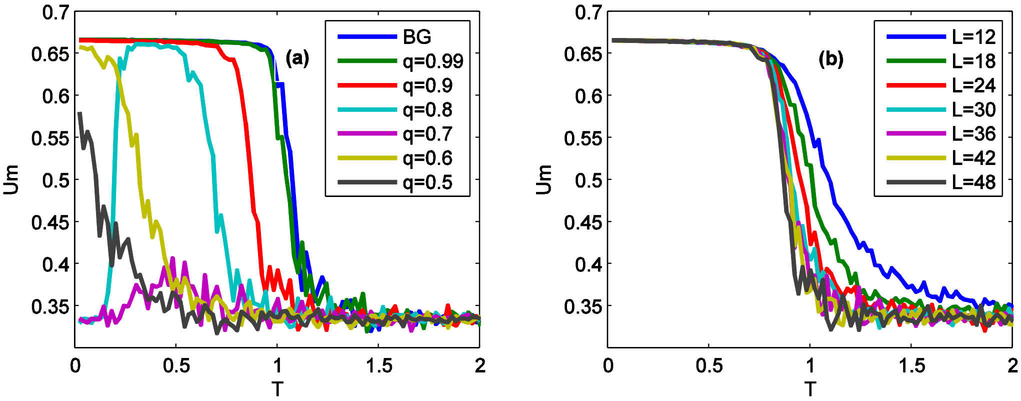

Figure 3 : Curves of variation of the Binder cumulant of the magnetization as a function of temperature in the case of the XY model for: **(a)** $L^2 = 48^2$ with different values of q and the case of the Boltzmann–Gibbs statistic (BG) , **(b)** $q = 0.9$ with different values of L.

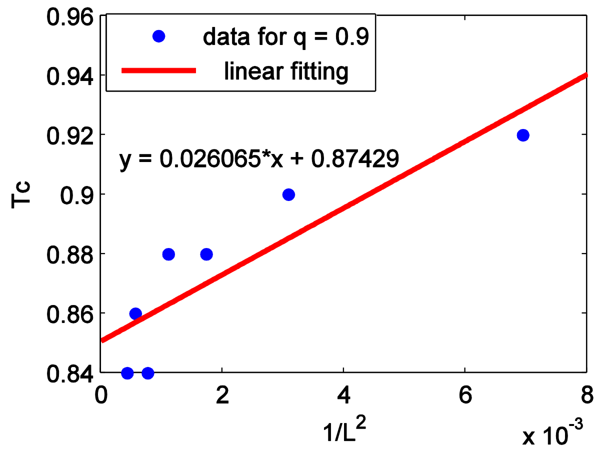

Figure 4 : Linear fitting of the critical temperature T_C as a function of the inverse of the lattice size $1/L^2$ for q = 0.9.

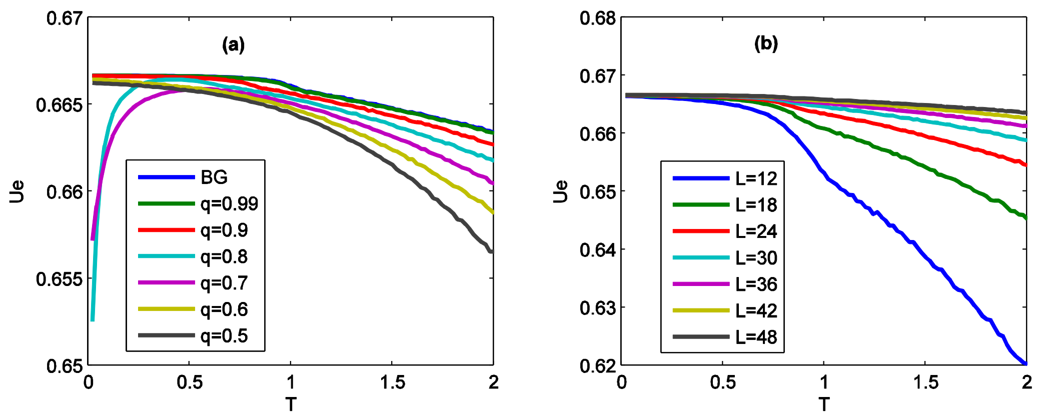

Figure 5 : Curves of variation of the Binder cumulant of energy as a function of temperature in the case of the XY model for: **(a)** $L^2 = 48^2$ with different values of q and the case of the Boltzmann–Gibbs statistic (BG), **(b)** q = 0.9 with different values of L.

Table 1 : Values of the critical temperature T_C, at the thermodynamic limit, estimated in the case of the Boltzmann-Gibbs statistic (BG) and in the case of the Tsallis statistic with different values of the entropic index q using: **(a)** the Binder cumulant of the magnetization method, **(b)** the linear fitting method.

	T_C	
	(a)	(b)
BG	0.96	1.04
$q = 0.99$	0.96	1.04
$q = 0.9$	0.74	0.87
$q = 0.8$	0.54	0.64