Nonextensivity and Tsallis statistics in magnetic systems

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We have studied the role of long-range interactions on the thermodynamics of magnetic systems. We have simulated, through the Monte Carlo method, magnetization curves of a two-dimensional classical Ising model including a long-range dipole-dipole-like interaction, where the range of interaction is tuned by a parameter α. Based on the conjectures of Tsallis statistics, we show that, for $\alpha/d \leqslant 1$ ($d=2$), the appropriate form of the equation of state is given by $M/N = m(T^*,H^*)$ with $T^* \equiv T/N^*$ and $H^* \equiv H/N^*$. The normalization factor $N^*[N^* \equiv (N^{(1-\alpha/d)}-1)/(1-\alpha/d)]$ emerges from the nonextensivity of thermodynamic variables of energy type. The crossover from nonextensive to extensive behavior at $\alpha/d=1$ occurs smoothly and similarly to other quite different systems, thus suggesting it to be a general result. [S0163-1829(97)06009-8]

In nature long-range spatial interactions or long-range memory effects may give rise to very interesting behaviors. Among them, one of the most intriguing arises in systems which, given the appropriate conditions of their thermodynamic variables, such as internal energy, magnetization, etc., are nonextensive (nonadditive). The best known examples of such systems are the gravitational N-body problem and astrophysics,[1] black holes and superstrings,[2] Lévy-like and correlatedlike anomalous diffusion,[3] two-dimensional turbulence,[4] granular matter, such as sandpile,[5] and many others. These systems share a very subtle property: they violate the Boltzmann-Gibbs (BG) statistics—the bridge to the equilibrium thermodynamics.

Inspired by multifractals concepts, Tsallis[6] has proposed a generalization of the BG statistical mechanics. He introduced an entropic expression characterized by an index q which leads to a nonextensive statistics,

$$S_q = k\frac{1-\Sigma_{i=1}^{W} p_i^q}{q-1}, \tag{1}$$

where p_i are the probabilities associated with the microscopic configurations, and W is their total number. The value of q is a measure of the nonextensivity of the system; $q=1$ corresponds to the standard, extensive, BG statistics. Indeed, using $p_i^{(q-1)} \sim 1+(q-1)\ln p_i$ in the limit $q \to 1$, we immediately verify that

$$S_1 = -k\sum_{i=1}^{W} p_i \ln p_i .$$

According to Tsallis conjectures, depending on the range of interactions and on the range of memory effects present in the system, the BG formalism may or may not fail. Usually, the range of interactions and memory effects are of the short-range type and the BG formalism is fully applied. For instance, models usually have *nearest-neighbor* interactions and their dynamic transition probabilities are of the Markov type; i.e., take *only* the previous state of the system in the computation. Before discussing the unusual case, it is important to note that in the scope of Tsallis statistics the order in which the limits in size (N) and in time (t) are taken, i.e., $\lim_{N\to\infty}\lim_{t\to\infty}$ and $\lim_{t\to\infty}\lim_{N\to\infty}$, may yield different results.[7] This is not the case of standard BG statistics, where due to the ergodic hypothesis the order of the limits in size and in time commute. For long-range interactions and memory effects, at the *equilibrium* state (i.e., $\lim_{N\to\infty}\lim_{t\to\infty}$) the BG formalism is only *weakly violated*, so that $q=1$ holds, but appropriated scaling functions must be added. Furthermore, for long-range interactions and memory effects, but now at the *metaequilibrium* state (i.e., $\lim_{t\to\infty}\lim_{N\to\infty}$), the BG formalism is *strongly violated* and $q \neq 1$. This is the case of the examples mentioned above.

The lack in the literature on this subject applied to magnetism has motivated us to discuss the role of long-range interactions in the thermodynamics of magnetic systems. In this paper, we deal with a generalized dipole-dipole interaction where the range of interaction is tuned by a parameter α. This is an example of the *weak violation* of the BG statistics.

Let us consider a magnetic system with N spins following a d-dimensional Ising long-range interaction potential Hamiltonian:

$$-\sum_{i,j}\left(\frac{J}{r_{ij}^{\alpha}}\right)\sigma_i\sigma_j, \tag{2}$$

where J is the exchange coupling constant ($J>0$), r_{ij} is the distance between the spins i and j, σ_i assumes the values ± 1, and α is the range of interaction ($0 \leqslant \alpha < \infty$). The internal energy per spin of the system is calculated integrating Eq. (2) over the volume[8]

$$\frac{E}{N} \propto \int_1^{N^{1/d}} \frac{r^{d-1}}{r^{\alpha}}\, dr = \frac{1}{d}\,\frac{N^{1-\alpha/d}-1}{1-\alpha/d}; \tag{3}$$

thus for large systems the energy per spin is given by

$$\frac{E}{N} \propto \left\{\begin{matrix} cte, & \alpha/d>1 \\ \ln N, & \alpha/d=1 \\ N^{1-\alpha/d}, & \alpha/d<1 \end{matrix}\right\}. \tag{4}$$

One easily observes that in the thermodynamic limit ($N \to \infty$) the energy per spin does not converge in the range

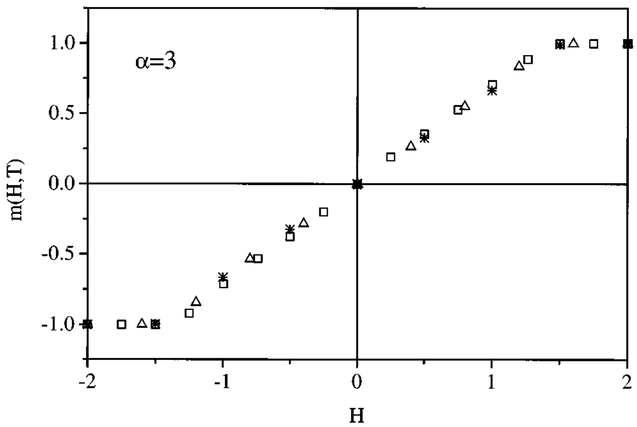

FIG. 1. Magnetization curves in the function of the magnetic field for a system size of 32×32 (□), 48×48 (△), and 64×64 (⋆) spins for the usual dipole-dipole interaction ($\alpha=3$) at $T=0.3$.

$0<\alpha/d\leqslant 1$. Nevertheless, defining $N^*\equiv(N^{(1-\alpha/d)}-1)/(1-\alpha/d)$ the convergence can be recovered normalizing the energy per spin also by N^*, i.e., E/NN^*. For $\alpha/d=1$, $N^*\propto \ln N$. Therefore, other thermodynamic variables of the energy type $(E,F,G\dots)$ scale with NN^*. In order to extend this reasoning to other thermodynamic quantities, one takes the Gibbs free energy expressed in thermodynamic variables with their conjugates and normalizes[9] by NN^*,

$$\frac{G}{NN^*}=\frac{U}{NN^*}-\frac{T}{N^*}\frac{S}{N}-\frac{H}{N^*}\frac{M}{N}+\frac{p}{N^*}\frac{V}{N}\dots \quad (5)$$

After rearranging the preview equation in a convenient way, it suggests that extensive quantities such as $S,M,V\dots$ scale with N, and intensive quantities in BG statistics such as $T,H,p\dots$ scale in Tsallis statistics with N^*. Hence, for $0<\alpha/d\leqslant 1$ the equation of state in magnetic systems would be $M/N=m(T^*,H^*)$ with $T^*\equiv T/N^*$ and $H^*\equiv H/N^*$. Indeed, since N^* is a constant for $\alpha/d>1$, we can always use the equation of state in this new form, i.e., for the entire range of α/d.

Now, let us consider a system in a two-dimensional $(d=2)$ square lattice taking a modified Ising Hamiltonian,

$$\mathcal{H}=-\sum_{\langle i,j\rangle}\sigma_i\sigma_j+0.5\sum_{i,j}\frac{\sigma_i\sigma_j}{r_{ij}^{\alpha}}-H\sum_i\sigma_i, \quad (6)$$

where σ_i assumes the values ± 1 on a site i. The first summation represents the exchange interaction acting upon nearest neighbors *only*, whereas the long-range interaction, represented by the second term, is summed over *all* pairs of neighbors. The Hamiltonian was normalized by J and the magnetic moment μ is fixed as 1. For $\alpha=3$, the long-range interaction corresponds to the usual dipole-dipole interaction. *The only parameter of the model is the range of interaction, characterized by the constant* α. The last term denotes the interaction between the spins and an external magnetic field (H). The exchange and the long-range interactions favor the spins alignment parallel and antiparallel, respectively, and with a prefactor 0.5 in the long-range interaction the system is a ferromagnet with stripe domains pointing up and down.[10]

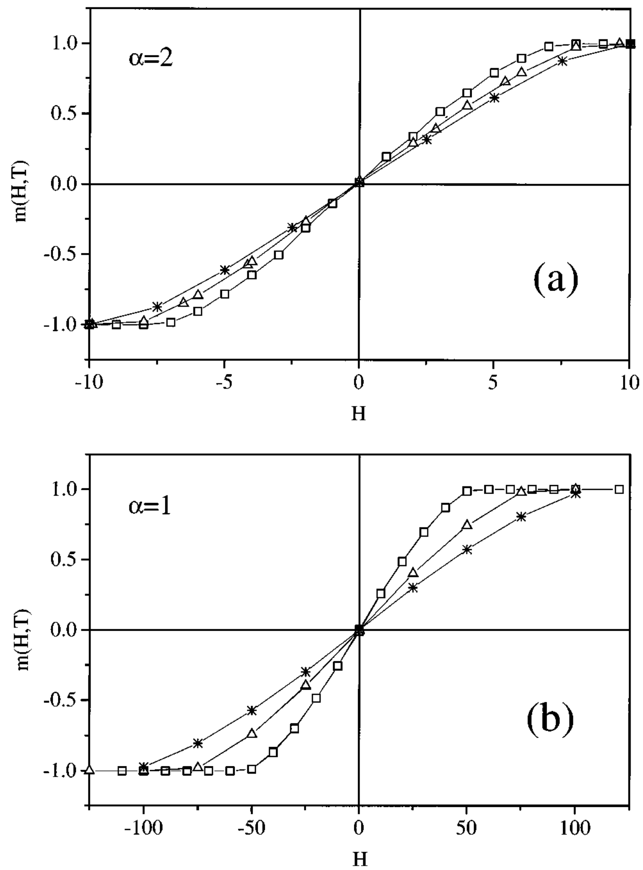

FIG. 2. Magnetization curves in the function of the magnetic field at $T=0.3$ for $\alpha=2$ (a) and $\alpha=1$ (b) (symbols as in Fig. 1).

We have simulated magnetization curves for lattice sizes of $L\times L$ spins with $L=32$,48, and 64, for different ranges of the long-range interaction α between 1 and 4 through the Monte Carlo method. We have used semiopen boundary conditions, that is, periodic for exchange interactions, and open for dipole-dipole interactions. This boundary condition produces the same results as obtained by the Ewald summation technique, however in a much reduced computing time (for further details, see Ref. 10). The magnetization curves were obtained at fixed temperature, starting from a saturation magnetic field. Thereafter, the field is decreased down to a negative saturation value passing through zero; at each magnetic-field value the number of Monte Carlo steps is large enough to ensure the system reaches the equilibrium. In the model, the equilibrium is stated in the sense, $\lim_{N\to\infty}\lim_{t\to\infty}$, i.e., the magnetization attains a stationary value at long times, and afterwards we analyze the influence of the system size.

We show in Fig. 1 the magnetization per spin for lattice sizes of 32×32,48×48 and 64×64 in the dipolar case $(\alpha=3)$, i.e., $\alpha/d>1$, at a temperature well below the critical temperature. Note that these sizes are large enough to prevent any finite-size effect which may arise from the simulation. We observe a superposition of all $m(H,T)$ curves as is expected in the BG statistics.

Now, changing the range of interaction to $\alpha=2$, i.e., $\alpha/d=1$, a surprising effect emerges from the $m(H,T)$ curves as shown in Fig. 2(a); the magnetization at a field lower than the saturation one decreases for larger system sizes, disap-

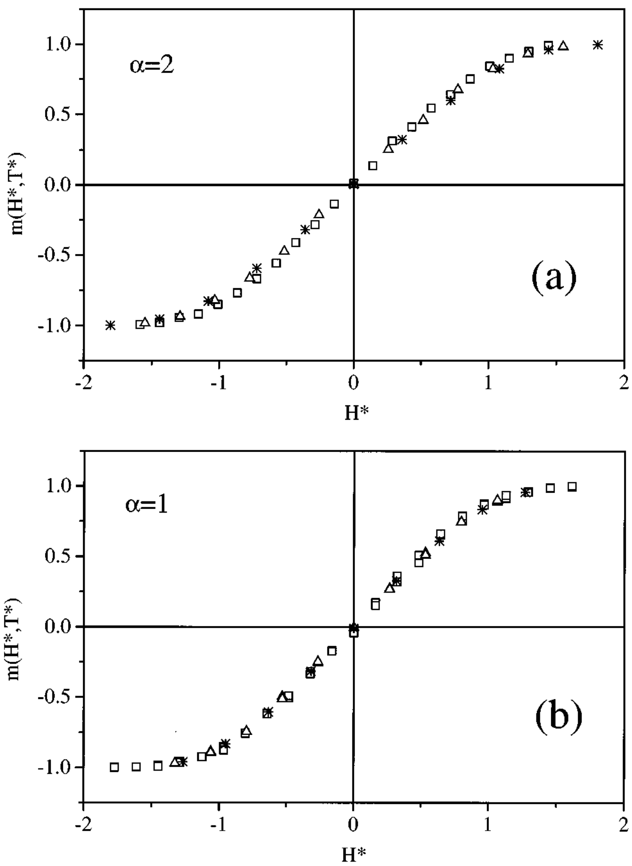

FIG. 3. Magnetization curves in the function of the variable H^* at $T^*=0.3$ for $\alpha=2$ (a) ($T_{\square}=2.08$, $T_{\triangle}=2.32$, and $T_{\star}=2.49$) and $\alpha=1$ (b) ($T_{\square}=18.6$, $T_{\triangle}=28.2$, and $T_{\star}=37.8$) (symbols as in Fig. 1).

pearing the superposition of the $m(H,T)$ curves as in the previous case ($\alpha=3$, see Fig. 1). Shown in Fig. 2(b) is the same picture, now for $\alpha=1$, i.e., $\alpha/d<1$. As discussed above, this is a consequence of the nonextensivity which arises from the long-range interactions in the range $\alpha/d\leqslant 1$, and H and T are no longer intensive quantities. We present in Figs. 3(a) and 3(b) the $m(H^*,T^*)$ curves for $\alpha=2$ and $\alpha=1$, respectively, now as a function of H^* and T^*. One observes that the scaling of both $m(H^*,T^*)$ curves for different system sizes is recovered. It suggests that the equation of state would be better expressed as $m(H^*,T^*)$ for the entire range of α ($0\leqslant\alpha/d<\infty$), i.e., for long-range and short-range interactions. At this point it is important to clarify that the real temperature of the system is the temperature of the thermal bath T, and the real applied magnetic field on the system is H. Nevertheless, the variables T^* and H^* are suitable to recover the same formalism used in BG statistics.

An interesting picture emerges plotting the $m(H^*,T^*)$ curves together below and above $\alpha=2$ ($\alpha/d=1$). Besides the fact that $m(H^*,T^*)$ is size independent for $\alpha/d\leqslant 1$, i.e., scale independently of the system size, the same scale occurs independently of α/d. As a consequence, all the $m(H^*,T^*)$ curves collapse *independently of size and of the α/d ratio*, as it is shown in Fig. 4. On the other hand, for $\alpha>2$ the slope of $m(H^*,T^*)$ curves at low field increases

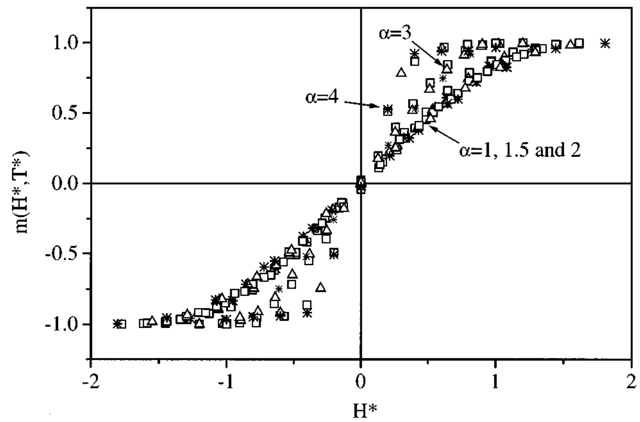

FIG. 4. Magnetization curves in the function of the variable H^* at $T^*=0.3$ for values of α below and above $\alpha/d=1$ ($\alpha=1,1.5,2,3$, and 4), $T_{\square}(\alpha=1)$, $T_{\triangle}(\alpha=1)$ and $T_{\star}(\alpha=1)$ same as Fig. 3(b); $T_{\square}(\alpha=1.5)=5.58$, $T_{\triangle}(\alpha=1.5)=7.11$ and $T_{\star}(\alpha=1.5)=8.4$; $T_{\square}(\alpha=2)$, $T_{\triangle}(\alpha=2)$, and $T_{\star}(\alpha=2)$ same as Fig. 3(a); $T_{\square}(\alpha=3)=0.49$, $T_{\triangle}(\alpha=3)=0.51$, and $T_{\star}(\alpha=3)=0.52$; $T_{\square}(\alpha=4)=T_{\triangle}(\alpha=4)=T_{\star}(\alpha=4)=0.29$ (symbols as in Fig. 1).

for increasing values of α. The insensitivity to α in the first regime ($\alpha/d\leqslant 1$), was also observed in molecular dynamics simulations using generalized Lennard-Jones potentials.[11] Indeed, this behavior is nothing else but a signature of the nonextensivity behavior which emerges from the long-range interactions.

In order to characterize the crossover from the nonextensive to the extensive behavior we show in Fig. 5 the susceptibility $[\chi\equiv\partial m(H^*,T^*)/\partial H^*)_{H^*=0}]$ at $T^*=0.3$, i.e., the slope of $m(H^*,T^*)$ curves at zero field, for different α values. We observe that the crossover occurs for $\alpha=2$ ($\alpha/d=1$), above which the susceptibility increases continuously without discontinuity on its first derivative relative to α. The same behavior has been observed in particles subject to long-range Lennard-Jones-like potentials.[11]

Summarizing, we have presented a simple model which

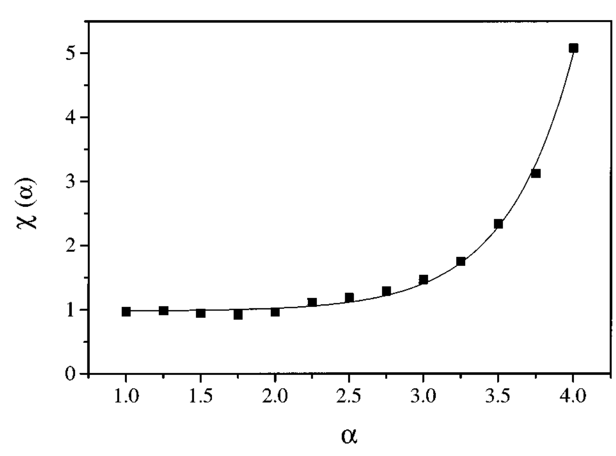

FIG. 5. Susceptibility $\chi(\alpha)$ taken at low fields at $T^*=0.3$ for $1\leqslant\alpha\leqslant 4$. The values of $T_{\square}(\alpha)$, $T_{\triangle}(\alpha)$, and $T_{\star}(\alpha)$ are the same as Fig. 4. The full line is a guide to the eyes.

shows a weak violation of the BG statistics, i.e., the nonextensive behavior of the thermodynamics variables (for instance, E,F,G,S, etc.) in the BG statistics framework $(q=1)$. Our results support the conjectures of Tsallis statistics. Furthermore, we observed that the crossover of the susceptibility at $\alpha/d=1$ from the nonextensive to the extensive regimes occurs smoothly, suggesting it to be a general behavior of systems which weakly violate the BG statistics.

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