Long-range interactions and nonextensivity in ferromagnetic spin models

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The Ising model with ferromagnetic interactions that decay as $1/r^{\alpha}$ is analyzed in the nonextensive regime $0 \leqslant \alpha \leqslant d$, where the thermodynamic limit is not defined. In order to study the asymptotic properties of the model in the $N \to \infty$ limit (N being the number of spins) we propose a generalization of the Curie-Weiss model, for which the $N \to \infty$ limit is well defined for all $\alpha \geqslant 0$. We conjecture that mean-field theory is *exact* in the last model for all $0 \leqslant \alpha \leqslant d$. This conjecture is supported by Monte Carlo heat-bath simulations in the $d=1$ case. Moreover, we confirm a recently conjectured scaling by Tsallis that allows for a unification of extensive ($\alpha > d$) and nonextensive ($0 \leqslant \alpha \leqslant d$) regimes.

It has been known for a long time that systems with long-range microscopic interactions can exhibit nonextensive behavior (see Refs. 1–3, among many others, and references therein). In other words, if the effective range of the interactions between the constituent particles decays slowly enough with the distance, the free energy $F = -\beta \ln Z$, with $Z \equiv \mathrm{Tr}\, \exp(-\beta H)$ (H being the Hamiltonian of the system and $\beta \equiv k_B T$) will grow *faster* than the number N of microscopic elements when $N \to \infty$ and the so-called thermodynamic limit will be not defined.

Besides their fundamental theoretical interest in physics, microscopic models with long-range interactions which decay slowly are of interest nowadays, in view of their relationship with neural systems modeling,[4] where far away localized neurons interact through an action potential that decays slowly along the axon. Other related problems are spin sytems with Ruderman-Kittel-Kasuya-Yosida- (RKKY) like interactions, which are present in spin glasses,[5] critical phenomena in highly ionic systems,[6] Casimir forces in fluid near the critical point,[7] kinetic Ising model,[8] and phase segregation in model alloys.[9] Many of these problems can be studied using some variation of the Ising model (e.g., Hopfield model of neural network, Edward-Anderson of spin glasses, etc.), or its lattice-gas version, as in model alloys.[9] Moreover, even systems not directly related with magnetic ones present often critical properties that fall in the universality class of some magnetic systems, the Ising model being the most simple nontrivial one. Hence, a deep comprehension of the general properties of the Ising model with long-range interactions is relevant to understand the behavior of this kind of system. As we will show, even the most simple case, i.e., the ferromagnetic model, presents nontrivial nonextensive behaviors and therefore it represents a good starting point to the study of more complex models.

In this paper we consider an Ising ferrromagnet with *long-range* interactions, that means, a system described by the Hamiltonian

$$H = -\sum_{(i,j)} J(r_{ij}) S_i S_j \quad (S_i = \pm 1 \ \ \forall i), \tag{1}$$

with

$$J(r_{ij}) = \frac{J}{r_{ij}^{\alpha}} \quad (J>0;\ \ \alpha>0), \tag{2}$$

where r_{ij} is the distance (in crystal units) between sites i and j, and where the sum $\Sigma_{(i,j)}$ runs over all distinct pairs of sites on a d-dimensional simple hypercubic lattice. The $\alpha \to \infty$ limit corresponds to the first-neighbor model. The $\alpha = 0$ limit corresponds, after a rescaling $J \to J/N$, to the Curie-Weiss model.

Let us introduce the sums $\phi_i(\alpha) = \Sigma_{j \neq i} J(r_{ij})$. A sufficient condition (and believed to be necessary[10]) for the existence of the thermodynamic limit of this system is that

$$\phi(\alpha) = \lim_{N \to \infty} \frac{1}{N} \sum_i \phi_i(\alpha) < \infty. \tag{3}$$

Let us now take a d-dimensional hypercube of side $L+1$ and $N = (L+1)^d$, and let $i=0$ be the central site of the hypercube. We have that

$$\phi(\alpha) = \lim_{N \to \infty} \phi_0(\alpha). \tag{4}$$

Then

$$\phi_0(\alpha) = J \sum_{i_1=1}^{L/2} \cdots \sum_{i_d=1}^{L/2} \frac{1}{(i_1^2 + i_2^2 + \cdots + i_d^2)^{\alpha/2}}. \tag{5}$$

Using the Euler-McLaurin sum formula[13] we can approximate, for $L \gg 1$,

$$\phi_0(\alpha) \approx J 2^d \int_1^{L/2} dx_1 \ \cdots \int_1^{L/2} dx_d \ \frac{1}{(x_1^2 + x_2^2 + \cdots + x_d^2)^{\alpha/2}}$$

$$\propto J \int_1^{L/2} dr\, r^{d-1-\alpha}.$$

Hence, $\phi_0(\alpha)$ shows the following asymptotic behavior for $N \gg 1$:

$$\phi_0(\alpha)\sim JC_d(\alpha)2^\alpha\begin{cases}\dfrac{1}{1-\alpha/d}(N^{1-\alpha/d}-1) & \text{if } \alpha\neq d,\\ \ln N & \text{if } \alpha=d.\end{cases} \tag{6}$$

.

In other words,

$$\lim_{N\to\infty}\frac{(1-\alpha/d)}{(N^{1-\alpha/d}-1)J2^\alpha}\phi_0(\alpha)=C_d(\alpha) \quad \text{for } \alpha\neq d, \tag{7}$$

and

$$\lim_{N\to\infty}\frac{\phi_0(d)}{J2^d\ln N}=C_d(d), \tag{8}$$

where $C_d(\alpha)$ is a continuous function of α independent of N, with $C_d(0)=1$. Therefore, the thermodynamic limit is well defined for $\alpha>d$ (where the system presents extensive behavior), while for $\alpha\leqslant d$ the system becomes nonextensive, the critical temperature becomes infinite, and the standard Maxwell-Boltzmann formalism cannot be applied.[11,12] The system undergoes a second-order phase transition at finite temperature for all $\alpha>d$ when[11] $d\geqslant 2$ and for $1\leqslant\alpha\leqslant 2$ when[14] $d=1$. For $\alpha\to d^+$, the critical temperature shows the following asymptotic behavior:[11]

$$k_BT_c\sim J\phi(\alpha). \tag{9}$$

We now introduce a model that generalizes the Curie-Weiss one. Such model is described by the Hamiltonian

$$H'=-\sum_{(i,j)}J'(r_{ij})S_iS_j \tag{10}$$

with

$$J'(r_{ij})=\frac{J(r_{ij})}{N^*(\alpha)2^\alpha}, \tag{11}$$

where

$$N^*(\alpha)=\frac{1}{1-\alpha/d}(N^{1-\alpha/d}-1), \tag{12}$$

which behaves as

$$N^*(\alpha)\sim\begin{cases}\dfrac{1}{\alpha/d-1} & \text{for } \alpha/d>1,\\ \ln N & \text{for } \alpha/d=1,\\ \dfrac{1}{1-\alpha/d}N^{1-\alpha/d} & \text{for } 0\leqslant\alpha/d\leqslant 1,\end{cases} \tag{13}$$

for $N\to\infty$. This model reduces to the Curie-Weiss one for $\alpha=0$ and to our original model Eq. (1) [after rescaling $J\to J(\alpha/d-1)/2^\alpha$] for $\alpha>d$. From Eqs. (3), (4), and (6) we see that the thermodynamic limit of this model is well defined *for all* $\alpha\geqslant 0$. We expect this system to show a phase transition at finite temperature for all $\alpha\geqslant 0$ when $d\geqslant 1$ and for $0\geqslant\alpha\geqslant 2$ when $d=1$.

The mean-field theory for this model predicts a critical temperature $k_BT_c'=JC_d(\alpha)2^\alpha$, which is *exact* for $\alpha=0$ and for $\alpha\to d^+$. Hence, *we conjecture the critical temperature reproduces exactly the mean-field prediction for all* $0\leqslant\alpha\leqslant d$. This conjecture is difficult to verify for $d>1$, since for systems with long-range interactions it is hard to obtain reliable numerical data for the exact critical temperature. In what follows we show that $C_1(\alpha)=1$ for $0\leqslant\alpha\leqslant 1$ and then we will test our conjecture through a Monte Carlo numerical simulation.

Let us consider the $d=1$ system. In this case $\phi_0=2J\Sigma_{n=1}^{L/2}(1/n^\alpha)$. Then, for $\alpha>1$ $\phi(\alpha)=2J\zeta(\alpha)$ [$\zeta(x)$ is the Riemann zeta function] and the critical temperature diverges as[14] $k_BT_c\sim 2J/(\alpha-1)$ for $\alpha\to 1^+$. Using the asymptotic behaviors[13]

$$\sum_{n=1}^{M}n^{-z}\sim\frac{M^{1-z}}{1-z} \quad \text{for } \mathrm{Re}(z)>-1 \text{ and } z\neq 1, \tag{14}$$

$$\sum_{n=1}^{M}\frac{1}{n}\sim\ln M, \tag{15}$$

for $M\to\infty$, we get for $\alpha<1$

$$\phi_0\sim\begin{cases}2^\alpha\dfrac{N^{1-\alpha}}{1-\alpha} & \text{for } 0\leqslant\alpha\leqslant 1,\\ 2\ln N & \text{for } \alpha=1\end{cases} \tag{16}$$

and

$$C_1(\alpha)=\begin{cases}1 & \text{for } 0\leqslant\alpha\leqslant 1,\\ \dfrac{\alpha-1}{2^{\alpha-1}}\zeta(\alpha) & \text{for } \alpha>1.\end{cases} \tag{17}$$

For $d=1$ the following necessary condition must be satisfied in order to have a finite critical temperature:[15]

$$\lim_{N\to\infty}\sum_{n=1}^{N}nJ(n)=\infty. \tag{18}$$

Using Eq. (14), we see that

$$\sum_{n=1}^{N}nJ'(n)\sim\frac{J}{N^*(\alpha)2^\alpha}\frac{N^{2-\alpha}}{2-\alpha}.$$

Hence, the critical temperature for $d=1$ will be finite $\forall 0\leqslant\alpha\leqslant 2$.

If we denote by u', s', and f' the energy, entropy and free energy per particle associated with the Hamiltonian H', i.e.,

$$f'(T)=\lim_{N\to\infty}-\frac{\beta}{N}\ln Z',$$

with $Z\equiv Tr_{\{S_i\}}\exp(-\beta H')$,

$$u'(T)=\lim_{N\to\infty}\frac{1}{N}\mathrm{Tr}_{\{S_i\}}H'\exp(-\beta H')$$

and

$$f'(T)=u'(T)-Ts'(T),$$

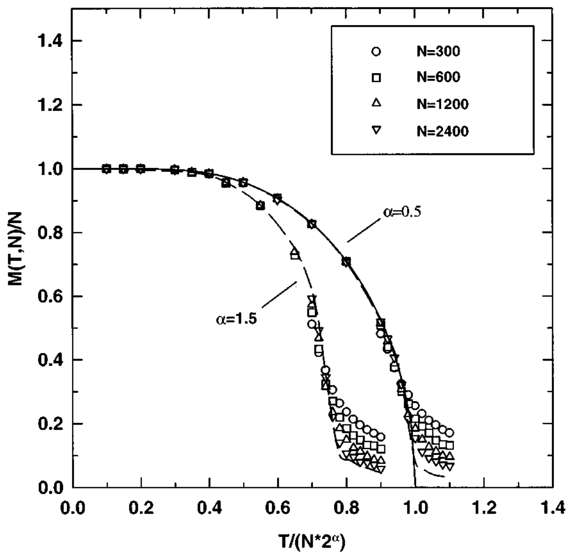

FIG. 1. Monte Carlo calculations of root mean square of the magnetization per spin $M(N,T)/N$ vs the scaled temperature $T/(N^*2^\alpha)$ using Hamiltonian (1), for $\alpha=0.5$, 1.5, and different values of the number of spins N in the one-dimensional lattice. In all cases the error bars are smaller than 0.01. The dashed lines are the $N=\infty$ extrapolation of $M(N,T)/N$. The extrapolated curves for $\alpha=0$, 0.25, and 0.75 are indistinguishable from the previous one. The solid line is the exact solution of the Curie-Weiss model.

we see that the generalized thermodynamic behavior associated with the Hamiltonian (1) can be accommodated, *for all* $\alpha\geqslant 0$, with the following scalings (in the limit $N\to\infty$ and for $T>0$):

$$U(N,T)\sim NN^*u'(T^*), \tag{19}$$

$$S(N,T)\sim Ns'(T^*), \tag{20}$$

$$F(N,T)\sim NN^*f'(T^*), \tag{21}$$

with $T^*\equiv T/N^*$, as was recently conjectured by Tsallis for general systems with long-range interactions.[17] Moreover, it can be easily shown that this type of scaling preserve the Legendre transformation structure of the thermodynamics, even in the long-range regime[17] $0\leqslant\alpha\leqslant d$. It is also expected that the magnetization $M\equiv\langle\Sigma_i S_i\rangle$ scales as $M(N,T)\sim Nm(T^*)$. Therefore, the suitable plot for looking for data collapse in a numerical simulation will be $M(N,T)/N$ vs T/N^*.

Let us consider the $d=1$ case. We performed a Monte Carlo simulation on a chain of N spins with Hamiltonian (1), using heat-bath dynamics, for $N=75$, 150, 300, 600, 1200, and 2400. We calculated the root mean square of the magnetization of the system $M(N,T)$ as a function of the temperature T for $\alpha=$ 0, 0.25, 0.5, 0.75, and 1.5. The results were averaged over K samples with different random number sequences ($K=100$, 50, 20, 20, 10, and 5 for $N=75$, 150, 300, 600, 1200, and 2400, respectively). For every value of α we obtained an extrapolated magnetization curve $M_\alpha(T)$, by performing a numerical extrapolation of $M(N,T)$ in $1/N$ to $N\to\infty$.

In Fig. 1 we show our results for $M(N,T)/N$ vs $T/(N^*\ 2^\alpha)$ for $\alpha=0.5$ and 1.5. These curves show clearly the data collapse above mentioned. Moreover, for $0\leqslant\alpha<1$ our results show that all curves $M_\alpha(T)$ *fall into a single one*, which coincides with the well-known exact solution for the Curie-Weiss model ($\alpha=0$ case), i.e., the solution of the equation $m=\tanh(m/T')$ $[m\equiv M/N;\ T'\equiv T/(N^*2^\alpha)]$. This last result is impressive. It does not only confirm our conjecture concerning the critical temperature ($T'_c=1$), but also shows that the full equation of state $m=m(T)$ at zero magnetic field becomes independent of α in the nonextensive regime $0\leqslant\alpha\leqslant 1$, suggesting that all the thermodynamic functions are those predicted by the mean-field theory. These results are consistent with recent Monte Carlo simulations of the correlation function, which reproduce the mean-field behavior in the same region[16] $0\leqslant\alpha\leqslant 1$.

In this paper we have found a scaling for the Ising model with long-range interactions that allows us to get a well-defined thermodynamic limit for any value of α. In particular, for $\alpha=0$, we recover the well-known Curie-Weiss scaling, which has been vastly used in the context of magnetic systems. With this scaling we were able to obtain the generalized thermodynamic behavior for $N\to\infty$ [Eqs. (19)–(21)] in the ferromagnetic case, which had been previously conjectured in a more general context by Tsallis.[17] It is worth stressing that with this scaling both extensive and nonextensive behaviors can be accommodated in a unified and elegant formalism and the (until now almost unexplored) $0\leqslant\alpha\leqslant d$ case becomes tractable. In the same way the nonextensive fully connected Ising model showed to be a very useful tool when suitable rescaled (Curie-Weiss model), we believe that the model here analyzed can represent not only a useful approach but also a more realistic one for certain problems such as neural networks and spin glasses among others.

On the other hand, due to the distance dependence of the interactions it becomes very difficult to obtain exact analytical results even in the $d=1$ case. We calculated the critical temperature in the mean-field approximation for any value of d and presented some numerical evidence that, (at least for $d=1$) not only does it reproduce the exact value in the whole nonextensive regime $0\leqslant\alpha\leqslant d=1$, but also the full magnetization curve $M(T)/N$ is given by the mean-field one. We believe that the critical temperature satisfies that property for all d. This conjecture is partially supported by the fact that it holds for $\alpha=0$ and $\alpha\to d^+$. Moreover, since the critical exponents are those of the mean-field theory both for $\alpha=0$ and $\alpha\to d^+$, we conjecture that all the critical properties will reproduce the mean-field behavior for $0\leqslant\alpha\leqslant d$. Monte Carlo simulations of the correlation function[16] for $d=1$ also support this statement. These results, although intuitive, are nontrivial and important, especially concerning spin glasses and biological systems (neural networks, immunology, etc) where a common approximation consists of considering fully connected models instead of the more realistic ones with slow decaying interactions (e.g., RKKY). Our results show that mean-field behavior is robust against variations of the range of the interactions α within the nonextensive region, at least for $d=1$. If our conjecture were true, this would have important practical implications: if you are considering systems with slow enough decaying interactions then you do not need sophisticated approximations, at least as far as critical properties are concerned.

It would be very interesting to extend the present analysis to more general systems of interacting particles with long-range interactions.

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