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Phase transitions in nonextensive spin systems

Robert Botet,[1] Marek Płoszajczak,[2] and Jorge A. González[3]
[1]*Laboratoire de Physique des Solides - CNRS, Bâtiment 510, Université Paris-Sud, Centre d'Orsay, F-91405 Orsay, France*
[2]*Grand Accélérateur National d'Ions Lourds (GANIL), CEA/DSM – CNRS/IN2P3, Boîte Postale 55027, F-14076 Caen Cedex, France*
[3]*Instituto Venezolano de Investigaciones Científicas, Centro de Física, Apartado 21827, Caracas 1020A, Venezuela*
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The spherical spin model with infinite-range ferromagnetic interactions is investigated analytically in the framework of nonextensive thermostatics generalizing the Boltzmann-Gibbs statistical mechanics. We show that for repulsive correlations, a weak-ferromagnetic phase develops. There is a tricritical point separating para-, weak-ferro, and ferro regimes. The transition from paramagnetic to weak-ferromagnetic phase is an unusual first-order phase transition in which a discontinuity of the averaged order parameter appears, even for finite number of spins. This result puts in a different way the question of the stability of critical phenomena with respect to the long-ranged correlations.

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Discussions of nonextensivity in thermodynamics go back to the 1970s [1]. Recently, nonextensive theories have become extremely important in several areas of physics [2]. However, there are still very important questions that should be addressed. The influence of the nonextensivity on phase transitions and their trace in finite systems is certainly a field that should be further explored [3]. In the collisions of atomic nuclei or charged atomic clusters, a highly excited nonequilibrium transient system is formed, which at a later stage of the reaction, approaches an equilibrium and splits into many fragments [4,5]. Observed signatures of criticality in these processes depend strongly not only on strong repulsive Coulomb interactions but also on the way the excited transient system is formed in collisions [6]. The fragility of those signatures manifests the inherently nonextensive character of these "critical phenomena" [7]. The general problem of the relation between critical behavior in small nonextensive statistical systems and the phase transitions in the thermodynamical limit is investigated here using the Berlin-Kac model (BKM) [8] in the framework of the Tsallis generalized statistical mechanics (TGSM) [9].

The TGSM was inspired by earlier works on nonextensive thermodynamics [1]. It is based on an alternative definition for the equilibrium entropy of a system whose ith microscopic state has probability $\hat{p}_i$ [9]

$$S_q = k\frac{1-\sum_i \hat{p}_i^q}{q-1}, \quad \sum_i \hat{p}_i = 1, \quad k>0, \tag{1}$$

and q (entropic index that is determined by the microscopic dynamics) defines a particular statistics. In the limit $q=1$, one obtains the usual Boltzmann-Gibbs (BG) formulation of the statistical mechanics. The main difference between the BG formulation and the TGSM lies in the nonadditivity of the entropy. For two independent subsystems A, B, such that the probability of $A+B$ is factorized into: $p_{A+B}=p_A p_B$, the global entropy verifies: $S_q(A+B)=S_q(A)+S_q(B)+(1-q)S_q(A)S_q(B)$. The entropy S_q has definite concavity for all values of q. In particular, it is always concave for $q>0$, and this is the case discussed in the present paper. It has been shown [11] that the TGSM retains much of the formal structure of the standard theory. Many important properties, such as the Legendre transformation structure of thermodynamics and the H-theorem (macroscopic time irreversibility) have been shown to be q invariant. Considering the fact that the essence of the second law of thermodynamics is concavity (see Ref. [13]), the mentioned properties of this entropy allow us to say that there are no problems with this law in TGSM.

The TGSM is relevant if the effective microscopic interactions are long ranged and/or the effective microscopic memory is long ranged and/or the geometry of the system is fractal [9,12,14]. In the superadditive regime $(1-q>0)$, independent subsystems A and B will tend to join together increasing in this way the entropy of the whole system. On the contrary, in the subadditive regime $(1-q<0)$, the system increases its entropy by fragmenting into separate subsystems. These ideas are in agreement with the results of Landsberg *et al.* [10,15] The subadditivity of entropy is expected when long-range repulsive interactions and correlations and/or long-range memory effects are present in the system [12,15]. This is in particular the relevant limit of the fragmentation of electrically charged (off-equilibrium) systems, such as those formed in the collisions of atomic nuclei or sodium clusters.

The BKM was introduced as an approximation of the Ising model. In the BKM, the individual spins are taken as continuous three-dimensional variables, but the rigid constraint on each local spin variable S_i (where $S_i=\pm 1/2$) in Ising model, is relaxed and replaced by an overall spherical constraint:

$$\sum_{i=1}^{i=N} S_i^2 = \frac{N}{4} \tag{2}$$

for N spins. In the present paper, we consider the infinite-range version of the BKM where all pairs of spins interact with the same strength, according to the Hamiltonian:

$$H=-\frac{J}{N}\sum_{(i,j)} S_iS_j-\frac{J}{8}. \tag{3}$$

The sum in Eq. (3) runs over all different pairs of spin indices (i,j). The constant term $-J/8$ is added to fix the origin of the energies at the vanishing total magnetization: $\Sigma_i S_i = 0$. The normalization of the ferromagnetic $(J>0)$ exchange energy as J/N, ensures finiteness of the energy per spin in an infinite system. The value of this energy should depend on the volume of the system.

One defines the magnetization per site by $\eta = N^{-1}\Sigma_i S_i$. Because of the inequality $(\Sigma S_i)^2 < N\Sigma S_i^2$, the value of η is contained in between $-1/2$ and $+1/2$. The phase of the system will be characterized by the average value of η^2, $m^2 = \langle \eta^2 \rangle$, where the brackets $\langle \cdots \rangle$ denote the ensemble average at a given temperature. The square root of m^2 plays the role of the order parameter.

The Hamiltonian of BKM may be expressed as a function of η:

$$H=-\frac{JN}{2}\eta^2, \tag{4}$$

and this allows us to obtain the degeneracy factor of the macroscopic states defined by the fixed number of spins N and the fixed energy E. The number of such states in the N-dimensional spin space is the volume of the intersection of the hypersphere (2) and of the hyperplane $\Sigma_i S_i = (-2NE/J)^{1/2}$. This intersection is a sphere of radius $(N/4+2E/J)^{1/2}$ in the $(N-1)$-dimensional space and its volume is $g_N(E)=a_N(1/4+2E/JN)^{N/2-1}$, where a_N is a numerical factor that depends only on the number of spins (system mass). Knowledge of this statistical weight, in addition to the energy given by Eq. (4) allows us to compute all thermodynamic quantities of the equilibrated system.

In BG statistical mechanics, the partition function is written in terms of the η distribution as

$$Z=A_0\int_0^{1/2}\eta \quad \exp[-Nf(\eta)]d\eta. \tag{5}$$

The constant A_0 is $2^{5-N}JNa_N\exp(-\beta J/8)$ and

$$f(\eta)=-\beta J\eta^2-(1-2/N)\ln(1-4\eta^2)/2$$

is the free energy per spin. In the limit $N\to\infty$, this function does not depend on N, which ensures the existence of the thermodynamic limit. Since this free energy is analytical in the variable η, $f(\eta)=[4(1-2/N)-\beta J]\eta^2/2+8(1-2/N)\eta^4+\cdots$, with a positive η^4 term and a change in sign of the η^2 term at the pseudocritical point $(\beta J)_{c,N}=4(1-2/N)$, the infinite system undergoes a second-order phase transition at the critical temperature $(\beta J)_c=4$. The critical exponents are given by the regular Landau-Ginzburg mean-field theory for the magnetic systems.

In the TGSM, the equilibrium energy distribution is given by [9]

$$p_{N,q}(E)=\frac{(1-\beta(1-q)E)^{1/(1-q)}}{Z_q}, \tag{6}$$

if $1-\beta(1-q)E>0$, and 0 otherwise. The partition function Z_q is defined by the normalization of $p_{N,q}$

$$\int g_N(E)p_{N,q}(E)dE=1. \tag{7}$$

All ensemble averages are then defined with respect to the properly normalized probability $p_{N,q}^q(E)g_N(E)$ [16]. For example, the averaged order parameter is given by

$$m_q^2\equiv\langle\eta^2\rangle_q=\frac{\int \eta^2(E)p_{N,q}^q(E)g_N(E)dE}{\int p_{N,q}^q(E)g_N(E)dE}. \tag{8}$$

Replacing the integration variable E by η, the value of m_q is

$$m_q^2=I_3/I_1, \tag{9}$$

with the integrals I_s defined by

$$I_s=\int_0^x \eta^s\left[1-\frac{\beta J\kappa}{2}\eta^2\right]^{-N/\kappa-1}(1-4\eta^2)^{N/2-1}d\eta, \tag{10}$$

and $x\equiv\min(1/2,\sqrt{2/\beta J\kappa})$ because of Eq. (6) and $|\eta|<1/2$. The fundamental parameter of the nonextensive generalization of the BKM is

$$\kappa=N(q-1) \tag{11}$$

instead of $q-1$. This parameter, which will be called hereafter the out-of-extensivity (OE) parameter, allows us to define the thermodynamic limit of the system in a natural way. Let us compare systems of different masses N such that the OE parameter (11) remains constant. In the relations (9) and (10), one may recognize the equivalent of a free energy per site

$$f_q(\eta)=\ln(1-\beta J\kappa\eta^2/2)/\kappa-\ln(1-4\eta^2)/2, \tag{12}$$

which is independent of N when κ is a constant. Existence of this free energy per spin implies, in turn, the existence of the thermodynamic limit in the system. For a fixed value of the OE parameter, the interesting values of q approach 1 as the number of spins increases.

When the number of spins N is finite, the integrals I_s may be expressed by the hypergeometric functions. At high temperatures $\beta J<8/\kappa$, the upper bound for η in Eq. (10) is 1/2. The integrand in this case is always finite, and m_q is a positive decreasing function of the temperature. Moreover, if $\kappa>2/(1-2/N)$, then for all these temperatures one has $\beta J<4(1-2/N)$ and $m_q\propto 1/\sqrt{N}$, similar to the standard paramagnetic phase. In particular, when $\beta J\to 8/\kappa$ by lower values, then the limiting value is $m_q=N^{-1/2}[\kappa/\{2(\kappa-2)\}]^{1/2}$. On the other hand, if $\kappa<2/(1-2/N)$, then this $1/\sqrt{N}$ behavior of m_q holds only when $\beta J<4(1-2/N)$. For higher val-

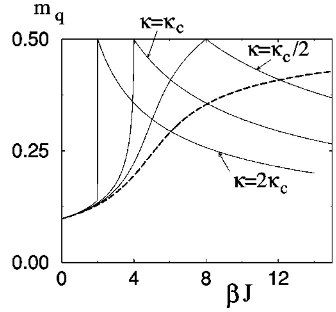

FIG. 1. Plots of the averaged magnetization of the infinite-range BKM in the TGSM for $N=50$ interacting spins and $\kappa=2\kappa_c, \kappa_c, \kappa_c/2$. κ_c is the value of the OE parameter for which the pseudocritical point of the standard second-order phase transition [here, $(\beta J)_{c,N}=3.84$] and the critical point for the nonextensive BKM ($(\beta J)_{c,q}=8/\kappa$) occur at the same temperature. The BG limit ($\kappa=0$) is shown by the dashed line.

ues of βJ, the leading behavior of the order parameter takes finite values independent of N, and tends to 1/2 when $\beta J\rightarrow 8/\kappa$ by the lower values.

At low temperatures, $\beta J>8/\kappa$, the quantities $[1-(\beta J\kappa/2)\eta^2]^{-N/\kappa-1}$ diverge for finite values of η smaller than 1/2, and the value of m_q is dominated by the behavior of the integrand near this divergency. In this case, $m_q=\sqrt{2/(\beta J\kappa)}$, since the order-parameter probability distribution collapses into the two Dirac distributions. Moreover, if βJ tends to $8/\kappa$ by larger values, the limit of m_q values is 1/2. This implies that if $\kappa>2/(1-2/N)$, then the averaged order parameter m_q has a discontinuous jump at the critical temperature $(\beta J)_{c,q}=8/\kappa$ between the small value of order $1/\sqrt{N}$ and 1/2. Otherwise, if $\kappa<2/(1-2/N)$, then m_q is continuous but its first temperature derivative becomes discontinuous at this critical temperature $(\beta J)_{c,q}=8/\kappa$, leading to the second-order critical phenomenon. Both behaviors are exemplified in Fig. 1. The tricritical point $[(\beta J)_{TC}=4,\kappa_{TC}=2]$ separates the phase boundary line in transitions of different nature (discontinuous/continuous). One of the continuous phase transitions is the simple continuation of the well-known paramagnetic ⇔ ferromagnetic transition for the BG statistics, while the other one is a second-order phase transition (ferromagnetic ⇔ weak-ferromagnetic) due to the presence of the long-range repulsive correlations/memory effects.

Since the above limiting temperatures and OE parameters do not depend on the mass N (the number of spins), the pattern of different behaviors of the order-parameter remains unchanged in the thermodynamic limit ($N\rightarrow\infty$) and one may draw the phase diagram $\beta J-\kappa$ ($\kappa>0$) (see Fig. 2). The first-order phase transition in the generalized BKM (the bold-face solid line in Fig. 2) remains unaltered in small systems, unlike the case of regular collective critical phenomena. The additional phase appearing on this diagram is due to the long-range nonextensive correlations that tend to disorganize spin coherence. This phase is called the weak-ferromagnetic state, because the order parameter in this state has a positive value, but this value is lowered by the disruptive long-range correlations (see Fig. 1 in the case $\kappa=\kappa_c/2$). This is the reason why the magnetization in the weak-ferromagnetic phase decreases when the temperature is lowered.

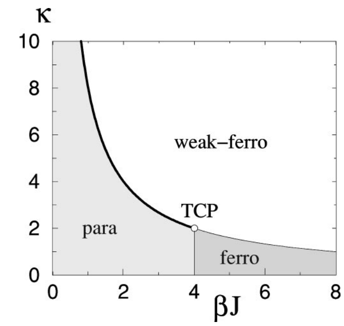

FIG. 2. Phase diagram of the infinite-ranged BKM ferromagnetic spin model in the TGSM at the thermodynamic limit. The bold-face solid curve shows the line where the first-order phase transition between paramagnetic and weak-ferromagnetic phase happens. For $0<\kappa<2$, the system undergoes two distinct second-order phase transitions: paramagnetic⇔ferromagnetic and ferromagnetic⇔weak-ferromagnetic. The tricritical point is located in $(\beta J)_{TC}=4$, $\kappa_{TC}=2$.

As we have seen above, the energy at constant volume in the BKM may be written as a function of the squared order parameter. This allows us to write the averaged energy as $U_q=-JNm_q^2/2$. The specific heat at constant mass and constant volume is the derivative of U_q with respect to the temperature, keeping the mass N and the coupling J fixed:

$$\frac{C_q}{k_B}=\frac{(\beta J)^2}{2}N\frac{\partial m_q^2}{\partial(\beta J)}. \tag{13}$$

From the above discussion, it is clear that there is a finite discontinuity of the specific heat when $\kappa<2/(1-2/N)$. But, there exists also a true divergence of C_q for the temperature $(\beta J)_{c,q}=8/\kappa$ when $\kappa\geqslant 2/(1-2/N)$, even if the system is finite.

There is some evidence [17] supporting the fact that long-range attractive interactions lead to $q<1$. We believe it is very important to stress that long-range repulsive interactions may lead to nonextensivity with $q>1$. The fact that the

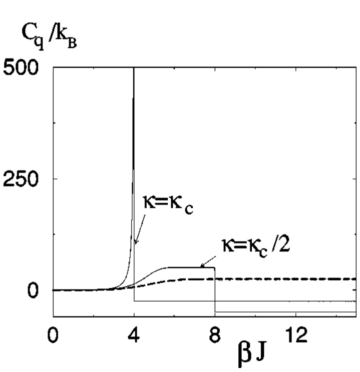

FIG. 3. Plots of the specific heat in the infinite-range BKM ($N=50$) for: $\kappa=\kappa_c$ [the divergence at $(\beta J)_{c,q}=8/\kappa$], and $\kappa=\kappa_c/2$ [the jump at $(\beta J)_{c,q}=8/\kappa$]. The BG limit ($\kappa=0$) is shown by the dashed line.

present system undergoes two different second-order phase transitions in the region $q>1$ is very remarkable. On the other hand, in this system, the fundamental parameter is $N(q-1)$ instead of q. This is a result in nonextensive physics.(See Fig. 3)

In conclusion, we have shown that the spherical spin model with long-range correlations/memory effects simulated in the framework of nonextensive thermostatistics, develops a weak-ferromagnetic phase in a subadditive entropy regime. An unusual first-order phase transition, which exhibits discontinuity of the order parameter even in finite systems, separates this phase from the standard paramagnetic phase. On the phase boundary line in the plane $\beta J-\kappa$, we have found the tricritical point separating the nature (discontinuous/continuous) of the transition. Above a critical value of the OE parameter, the spin system freezes into the weakly ordered (weak-ferromagnetic) phase, passing through the phase boundary in the discontinuous transition. For a fixed value of the OE parameter, the thermodynamic limit ($N\rightarrow\infty, q-1\rightarrow 0_+$) of the spin system differs from its BG limit. The nonextensivity shields the system from the continuous disorder⇔order phase transition and suggests that, in general, the second-order critical phenomena may be unstable in the presence of long-range repulsive correlations. This result puts in a different perspective the discussion of a ‘‘critical behavior’’ in collisions of atomic nuclei or atomic clusters, showing that the observed signals correspond possibly to a different limiting behavior than previously supposed.

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