Phase Transitions in Non-extensive Spin Systems

Robert Botet†, Marek Ploszajczak‡ and Jorge A. González*

† Laboratoire de Physique des Solides - CNRS, Bâtiment 510, Université Paris-Sud, Centre d’Orsay, F-91405 Orsay, France
‡ Grand Accélérateur National d’Ions Lourds (GANIL), CEA/DSM – CNRS/IN2P3, BP 55027, F-14076 Caen Cedex, France

* Instituto Venezolano de Investigaciones Científicas, Centro de Física, Apartado 21827, Caracas 1020A, Venezuela

The spherical spin model with infinite-range ferromagnetic interactions is investigated analytically in the framework of non-extensive thermostatics generalizing the Boltzmann-Gibbs statistical mechanics. We show that for repulsive correlations, a new 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 new way the question of the stability of critical phenomena with respect to the long-ranged correlations.

Discussion of nonextensivity in thermodynamics go back to 70’s [10]. Recently, non-extensive 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 non-extensivity on phase transitions and their trace in finite systems is certainly a field which should be further explored [3]. In the collisions of atomic nuclei or charged atomic clusters, a highly excited non-equilibrium transient system is formed in collisions [4]. Observed signatures of criticality in these processes depend strongly not only on strong repulsive Coulomb interactions but also on on the way the excited transient system is formed in collisions [3]. The fragility of those signatures manifests the inherently non-extensive character of these ‘critical phenomena’ [3]. The general problem of the relation between critical behavior in small non-extensive 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 non-extensive thermodynamics, going back to the 60’ [10], it is based on an alternative definition for the equilibrium entropy of a system whose entropy ver-

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

and \( q \) (entropic index which 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 [12] 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. [14]), 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 [13]. 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. [11-14]. The subadditivity of entropy is expected when long-range repulsive interactions and correlations and/or long-range memory effects are present in the system [13-14].

This is in particular the relevant limit of the fragmentation of electrically charged (off-equilibrium) systems, such as formed in the collisions of atomic nuclei or sodium clusters.

The BKM was introduced as an approximation of Ising model. In the BKM, the individual spins are taken as continuous 3-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 :

\[ \sum_{i=1}^{N} S_i^2 = \frac{N}{4} \]  

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

$$H = -\frac{J}{N} \sum_{\langle i,j \rangle} S_i S_j - \frac{J}{8} \sum_{i} S_i S_i^2$$  \hspace{1cm} \text{(3)}$$

The sum in (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: $\sum_i S_i = 0$. 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: $\eta = N^{-1} \sum_i S_i \cdot$. Because of the inequality: $(\sum S_i)^2 < N \sum S_i^2$, the value of $\eta$ is contained in between $-1/2$ and $+1/2$. The phase of the system will be characterized by the average value of $\eta^2$: $m^2 = < \eta^2 >$, where the brackets $< \cdots >$ 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 can be expressed as a function of $\eta$:

$$H = -\frac{JN}{2} \eta^2 \hspace{1cm} \text{(4)}$$

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 (4) and of the hyperplane: $\sum_i S_i = (-2NE/J)^{1/2}$. 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 which depends only on the number of spins (system mass). Knowledge of this statistical weight, in addition to the energy given by (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 $\eta$-distribution as:

$$Z = A_0 \int_0^{1/2} \eta \exp(-Nf(\eta))d\eta \hspace{1cm} \text{(5)}$$

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 $\eta$: $f(\eta) = 4(1-2/N) - \beta J\eta^2/2 + 8(1-2/N)\eta^4 + \cdots$, with a positive $\eta^2$-term and a change in sign of the $\eta^4$-term at the pseudo-critical 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 (6):

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

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

$$\int g_N(E)p_{N,q}(E)dE = 1 \hspace{1cm} \text{(7)}$$

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

$$m_q^2 = \frac{\int \eta^2(E)p_{N,q}^*(E)g_N(E)dE}{\int p_{N,q}^*(E)g_N(E)dE} \hspace{1cm} \text{(8)}$$

Replacing the integration variable $E$ by $\eta$, the value of $m_q$ is:

$$m_q^2 = I_3/I_1 \hspace{1cm} \text{(9)}$$

with the integrals $I_s$ defined by:

$$I_s = \int_0^x \eta^s [1 - \frac{\beta J\kappa}{2} \eta^2]^{N-1} (1-4\eta^2)^{N/2-1}d\eta \hspace{1cm} \text{(10)}$$

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

$$\kappa = N(q-1) \hspace{1cm} \text{(11)}$$

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 [17] remains constant. In the relations (6) and (10), one can recognize the equivalent of a free energy per site:

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

which is independent of $N$ when $\kappa$ is a constant. Existence of this free energy per spin implies in turn 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 $I_s$ can be expressed by the hypergeometric functions. At high temperatures: $\beta J < 8/\kappa$, the upper bound for $\eta$ in (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 \( m_q \propto 1/\sqrt{N} \), similarly 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 values of \( \beta J \), the leading behaviour of the order parameter takes finite values independent of \( N \), and tends to \( 1/2 \) when \( \beta J \to 8/\kappa \) by the lower values.

![Plot of the averaged magnetization of the infinite-range BKM in the TGS for N = 50 interacting spins and \( \kappa = 2\kappa_c, \kappa_c/2, \kappa_c \) is the value of the OE parameter for which the pseudo-critical point of the standard second order phase transition (here \( \langle \beta J \rangle_c,N = 3.84 \)) and the new critical point for the non-extensive BKM \( \langle \beta J \rangle_c,q = 8/\kappa \) occur at the same temperature. The BG limit (\( \kappa = 0 \)) is shown by the dashed line.](image)

At low temperatures: \( \beta J > 8/\kappa \), the quantities \( [1-(\beta J\kappa/2)\eta^2]^{-N/\kappa-1} \) diverge for finite values of \( \eta \) 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 \( \beta J \) 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 \( \langle \beta J \rangle_c,q = 8/\kappa \) 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 \( \langle \beta J \rangle_c,q = 8/\kappa \), leading to the second order critical phenomenon. Both behaviors are exemplified in Fig. 1. The tricritical point \( ((\beta J)_TCP = 4, \kappa_TCP = 2) \) 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 \( \Leftrightarrow \) ferromagnetic transition for the BG statistics, while the other one is a new second order phase transition (ferromagnetic \( \Leftrightarrow \) weak-ferromagnetic) due to the presence of the long-range repulsive correlations/memory effects.

![Phase diagram of the infinite-ranged BKM ferromagnetic spin model in the TGS 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\( \Leftrightarrow \)ferromagnetic and ferromagnetic\( \Leftrightarrow \)weak-ferromagnetic. The tricritical point is located in \( (\beta J)_TCP = 4, \kappa_TCP = 2 \).](image)

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 (\( N \to \infty \)) 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 non-extensive correlations which 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.

As we have seen above, the energy at constant volume in the BKM can be written as a function of the squared order parameter. This allows us to write the averaged energy as: \( U_q = -JN m_q^2/2 \). 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:

\[
\frac{C_q}{k_B} = \frac{(\beta J)^2}{2} N \frac{\partial m_q^2}{\partial (\beta J)}
\]

\[ (13) \]

\( \text{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 $\kappa \geq 2/(1 - 2/N)$, even if the system is finite.

![Graph](image_url)

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.

There is some evidence 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 can lead to non-extensivity with $q > 1$. The fact that the 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 new result in non-extensive physics.

In conclusion, we have shown that the spherical spin model with long-range correlations/memory effects simulated in the framework of non-extensive thermostatistics, develops a new 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 ($N \to \infty$, $q - 1 \to 0_+$) of the spin system differs from its BG limit. The non-extensivity shields the system from the continuous disorder $\Leftrightarrow$ 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 sig-

[1] A. Renyi, Probability theory (North-Holland, Amsterdam, 1970); Z. Daroczy, Information and Control 16, 36 (1970); L. Galgani and A. Scotti, Pure and Applied Chemistry 22, 229 (1970); P. T. Landsberg, Pure and Applied Chemistry 22, 215 (1970); J. Aczel and Z. Daroczy, On measures of information and their characterization (Academic Press, New York, 1975);
[2] R. Salazar and R. Toral, Phys. Rev. Lett. 83, 4233 (1999); F. Tamarit and C. Anteneodo, Phys. Rev. Lett. 84, 208 (2000); M. Buiatti, P. Grigolini, and A. Montagnini, Phys. Rev. Lett. 82, 3383 (1999); D. B. Walton and J. Rafelski, Phys. Rev. Lett. 84, 31 (2000);
[3] F. D. Nobre and C. Tsallis, Physica A 213, 337 (1995)
[4] J.P. Bondorf et al., Phys. Rep. 257, 133 (1995).
[5] F. Chandezon et al., Phys. Rev. Lett. 74, 3784 (1995); G. Seifert, R. Gutierrez and R. Schmidt, Phys. Lett. A 211, 357 (1996).
[6] J. Pochodzalla et al., Phys. Rev. C 55, 2991 (1997); Y.G. Ma et al., Phys. Lett. B 390, 41 (1997); Z. Majka et al., Phys. Rev. C 55, 2991 (1997); M. D’Agostino et al., Nucl. Phys. A 650, 329 (1999).
[7] K.K. Gudima et al., Phys. Rev. Lett. 85, 4691 (2000).
[8] T.H. Berlin and M. Kac, Phys. Rev. 86, 821 (1952).
[9] C. Tsallis, J. Stat. Phys. 52, 479 (1988).
[10] A. Renyi, Probability theory (North-Holland, Amsterdam, 1970); Z. Daroczy, Information and Control 16, 36 (1970); L. Galgani and A. Scotti, Pure and Applied Chemistry 22, 229 (1970); P. T. Landsberg, Pure and Applied Chemistry 22, 215 (1970); J. Aczel and Z. Daroczy, On measures of information and their characterization (Academic Press, New York, 1975);
[11] P. T. Landsberg and D. Tranah, Collective Phenomena 3, 73 (1980); D. Tranah and P. T. Landsberg, Collective Phenomena 3, 81 (1980).
[12] A. M. Mariz, Phys. Lett. A 165, 409 (1992); J. D. Ramshaw, Phys. Lett. A 175, 169; L. Borland, A. R. Plastino and C. Tsallis, J. Math. Phys. 39, 6490 (1998).
[13] C. Tsallis, Physica A 221, 277 (1995).
[14] B. H. Lavenda and J. Dunning-Davies, Found. Phys. Lett. 3, 435 (1990); B. H. Lavenda, Statistical physics: A probabilistic approach (Wiley, New York, 1991) (and see also the references cited there)
[15] K.T. Waldey and H.M. Urbassek, Physica A 176, 325 (1991).
[16] P. T. Landsberg and R. B. Mann, Class. Quantum Grav. 10, 2373 (1993).
[17] C. Tsallis, R.S. Mendes and A.R. Plastino, Physica A 261, 534 (1998).
[18] P. J. Jund, S. G. Kim, and C. Tsallis, Phys. Rev. B 52, 50 (1995); B. A. Mello et al. Phys. Lett. A 244, 277 (1998).