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Spin waves in a complex magnetic system: a nonextensive approach

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Abstract. In this paper we analyse the spin wave excitations (magnons) of an inhomogeneous spin system within the Boltzmann–Gibbs framework and then connect the results with the nonextensive approach (in the sense of Tsallis statistics). Considering an equivalence between those two frameworks, we can connect the entropic parameter q with moments of the distribution of exchange integrals of the inhomogeneous system. This supports the idea that the entropic parameter is connected to the microscopic properties of the system.

Keywords: heterogeneous materials (theory), new applications of statistical mechanics

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Contents

1. Introduction

Inspired by multifractals, Tsallis proposed a generalization of the Boltzmann–Gibbs entropy (S_{BG}) [1]

$$S_q = k\frac{1-\sum_i p_i^q}{q-1} \qquad (q \in \Re) \tag{1}$$

where q is the entropic parameter for a specific system and is connected to its dynamics, as recently proposed [2, 3], p_i are the probabilities satisfying $\sum_i p_i = 1$, k is a constant, and $\lim_{q\to 1} S_q = S_{\mathrm{BG}}$. This entropy for a system composed of two independent parts A and B, such as the probability is given by $P(A\bigcap B) = P(A)\,P(B)$, has the interesting property of nonextensivity (see for example [4, 5]):

$$S_q(A+B) = S_q(A) + S_q(B) + (1-q)S_q(A)S_q(B). \tag{2}$$

Besides representing a generalization, S_q, like S_{BG}, is non-negative, concave, and Lesche stable ($\forall\, q > 0$), and recently it has been shown that it is also *extensive* for some sorts of correlated systems [6].

Tsallis statistics, or nonextensive statistics, attempts to handle some anomalies that appear in physical problems which cannot be treated with Boltzmann–Gibbs (BG) statistics, for instance, long-range correlations, intrinsic cooperativity, multifractal structure, dissipation on a mesoscopic scale, strong non-Markovian microscopic memory [7]. These anomalies have the common characteristic of presenting power laws, instead of the ordinary exponential laws, which is also a characteristic of some complex systems. Its applicability ranges from protein folding [8] to financial markets [9], and from turbulence [10] to cosmic rays [11]. For example, in condensed matter problems we can cite Ising ferromagnets, Landau diamagnetism, electron–phonon systems, tight-binding-like Hamiltonians, metallic and superconductor systems [12]. In addition, an interesting example appears in [13, 14] where the authors predicted some peculiar magnetic

J. Stat. Mech. (2007) P08011

properties of manganites using nonextensive statistics like nanoscale inhomogeneity and phase coexistence, fractal structures, and long-range interactions [15]–[17].

Herein, we present some results comparing an inhomogeneous spin system within the BG framework and a homogeneous spin system in a nonextensive approach. This comparison led us to a connection between the nonextensive parameter q and specific moments of the distribution of the exchange integral of the inhomogeneous system. Thus, the spin waves in a inhomogeneous magnetic media can be described using nonextensive statistics and the entropic parameter is connected to the microscopic properties of the system, as previously shown for other systems by Beck [18], Beck and Cohen [19], Wilk and Włodarczyk [20], Reis *et al* [2], and therefore can be seen as a measurement of its complexity.

2. Spin waves

2.1. Magnons within an inhomogeneous medium: the Boltzmann–Gibbs framework

In a ferromagnet at $T = 0$ K all the spins have the maximum projection S in the z direction; this is the ground state configuration [21, 22]. Letting the spin system be in thermal contact with a reservoir, as the temperature increases, it will leave its ground state, the projections along the quantization direction will be reduced, and a wave-like perturbation will flow through the spin system; that is the spin wave (magnons). The spin wave theory leads to the description of the magnetism of ferromagnets at low temperatures, in the regime where the total angular momentum is close to its the projection in the z direction, $S \cong S^z$.

We will consider a system of N spins, each one interacting with z neighbours in an inhomogeneous way, and in the presence of a magnetic field B_0. Thus, the Hamiltonian for this inhomogeneous magnetic system is given by [21, 23, 24]

$$\mathcal{H} = -\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\, \mathbf{S}_\mathbf{R} \cdot \mathbf{S}_{\mathbf{R}+\mathbf{d}} - h \sum_{\mathbf{R}} S_{\mathbf{R}z} \tag{3}$$

in which $J_d(\mathbf{R}) > 0$ (always ferromagnetic) describes the inhomogeneity of the media, i.e., there is a distribution of exchange interactions $f(J)$, and $h = g\,\mu_\mathrm{B}\,B_0$ is the applied magnetic field. The whole Hamiltonian can be rewritten in terms of the collective motion operators in order to give us the magnetization per unit of volume. One can write the spin operators as

$$\mathbf{S}_\mathbf{R} \cdot \mathbf{S}_{\mathbf{R}+\mathbf{d}} = \tfrac{1}{2}\left[S^+_\mathbf{R} S^-_{\mathbf{R}+\mathbf{d}} + S^-_\mathbf{R} S^+_{\mathbf{R}+\mathbf{d}}\right] + S_{\mathbf{R}z} S_{\mathbf{R}+\mathbf{d}z}. \tag{4}$$

The Holstein–Primakoff transformation of spin operators, at low temperatures, is given by

$$S^+_\mathbf{R} \approx \sqrt{2\,S}\, a_\mathbf{R} \qquad \text{and} \qquad S^-_\mathbf{R} \approx \sqrt{2\,S}\, a^+_\mathbf{R} \tag{5}$$

in which $a^+_\mathbf{R}$ and $a_\mathbf{R}$ obey the commutation relation $[a_\mathbf{R}, a^+_\mathbf{R}] = 1$. The operators $a_\mathbf{R}$ and $a^+_\mathbf{R}$ can be written in terms of the collective motion of the system:

$$a_\mathbf{R} = \frac{1}{\sqrt{N}} \sum_k \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}}\, b_k \qquad \text{and} \qquad a^+_\mathbf{R} = \frac{1}{\sqrt{N}} \sum_k \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}}\, b^+_k \tag{6}$$

in which $[b_k, b^+_k] = 1$.

J. Stat. Mech. (2007) P08011

Thus, one can rewrite the exchange term of the Hamiltonian (3) as

$$-\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\,\mathbf{S}_{\mathbf{R}}\cdot\mathbf{S}_{\mathbf{R}+\mathbf{d}} = -\tfrac{1}{2}\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\,\left[S^{+}_{\mathbf{R}}S^{-}_{\mathbf{R}+\mathbf{d}} + S^{-}_{\mathbf{R}}S^{+}_{\mathbf{R}+\mathbf{d}}\right] - \sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\,S_{\mathbf{R}z}S_{(\mathbf{R}+\mathbf{d})z}. \tag{7}$$

Using the low temperature Holstein–Primakoff transformation, in terms of the collective motion operators, we have

$$\frac{1}{2}\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\left[S^{+}_{\mathbf{R}}S^{-}_{\mathbf{R}+\mathbf{d}} + S^{-}_{\mathbf{R}}S^{+}_{\mathbf{R}+\mathbf{d}}\right] = \sum_k \left(\frac{2\,S}{N}\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\cos(\mathbf{k}\cdot\mathbf{d})\right) b^{+}_k\,b_k \tag{8}$$

and

$$\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\,S_{\mathbf{R}z}S_{\mathbf{R}+\mathbf{d}z} = N\,S^2\left(\frac{1}{N}\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\right) - 2\,S\left(\frac{1}{N}\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\right)\sum_k b^{+}_k\,b_k \tag{9}$$

and note that we exclude the magnon–magnon interaction, represented by the term $n_k\,n_k$.

In terms of these operators,

$$S_{\mathbf{R}z} = S - a^{+}_{\mathbf{R}}a_{\mathbf{R}} \tag{10}$$

where S is the spin value per site and therefore the second term of the Hamiltonian can be written as

$$-h\sum_{\mathbf{R}} S_{\mathbf{R}z} = h\sum_k b^{+}_k\,b_k - h\,N\,S \tag{11}$$

where N is the number of sites. Hence, the Hamiltonian becomes

$$\mathcal{H} = -(h\,N\,S + N\,S^2\,J) + \sum_k\left(h + 2\,S\,J - \frac{2\,S}{N}\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\cos(\mathbf{k}\cdot\mathbf{d})\right) n_k \tag{12}$$

where $n_k = b^{+}_k\,b_k$ is the boson number operator and $J \equiv 1/N\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})$. The first two terms represent the fundamental state of the system, or the total energy without excitations. The term that describes the magnons is the second one. It has the form $\sum_k \hbar\,\omega_k\,n_k$ and gives the dispersion relation for this inhomogeneous magnetic system

$$\hbar\,\omega_k = h + 2\,S\,J - \frac{2\,S}{N}\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\cos(\mathbf{k}\cdot\mathbf{d}). \tag{13}$$

For large wavelength, one may write

$$\sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})\cos(\mathbf{k}\cdot\mathbf{d}) \approx \sum_{\mathbf{R},\mathbf{d}} J_d(\mathbf{R})[1 - \tfrac{1}{2}(\mathbf{k}\cdot\mathbf{d})^2] \tag{14}$$

and $(\mathbf{k}\cdot\mathbf{d})^2 = k^2\,a^2$, where a is the lattice parameter. Thus, the dispersion relation is

$$\hbar\,\omega_k \approx h + k^2\,\mathcal{D}(J) \tag{15}$$

where $\mathcal{D}(J) = a^2\,z\,S\,J$ is the stiffness parameter and z is the number of first neighbours.

As the interaction varies between spins, one may consider that it has a distribution $f(J)$. Thus, the average magnetization change, with respect to the saturation value of

J. Stat. Mech. (2007) P08011

the magnetization, per unit of volume is given by

$$\langle \Delta m \rangle = \frac{g\,\mu_{\rm B}}{2\,\pi^2} \int_0^\infty {\rm d}J\, f(J) \int_0^\infty {\rm d}k\, k^2 \langle n_k \rangle_J \tag{16}$$

where $\langle n_k \rangle_J$ is the Planck distribution. Thus (16) becomes

$$\langle \Delta m \rangle = \frac{g\,\mu_{\rm B}}{2\,\pi^2} \int_0^\infty {\rm d}J\, f(J) \int_0^\infty {\rm d}k\, \frac{k^2}{{\rm e}^{(k^2\,\mathcal{D}(J)+h)/k_{\rm B}\,T} - 1} \tag{17}$$

$$= \frac{g\,\mu_{\rm B}}{4\,\pi^2} \int_0^\infty {\rm d}J\, f(J) \frac{k_{\rm B}\,T}{\mathcal{D}(J)^{3/2}} \int_{h/k_{\rm B}\,T}^\infty {\rm d}x\, \frac{(k_{\rm B}\,T\,x - h)^{1/2}}{{\rm e}^x - 1} \tag{18}$$

where $x = (k^2\,\mathcal{D}(J) + h)/k_{\rm B}\,T$.

For $B_0 = 0$, i.e., $h = 0$, the inner integral becomes

$$\int_0^\infty \frac{x^{1/2}\,{\rm d}x}{{\rm e}^x - 1} = \frac{\sqrt{\pi}}{2} \zeta(3/2) \tag{19}$$

where $\zeta(n)$ is the Riemann zeta function. The volume magnetization variation due to magnon excitation of an inhomogeneous system is then given by

$$\langle \Delta m \rangle = \frac{\zeta(3/2)\,g\,\mu_{\rm B}}{8\,\pi^{3/2}} \left(\frac{k_{\rm B}\,T}{a^2\,z\,S}\right)^{3/2} \int_0^\infty {\rm d}J\, \frac{f(J)}{J^{3/2}} = \frac{\zeta(3/2)\,g\,\mu_{\rm B}}{8\,\pi^{3/2}} \left(\frac{k_{\rm B}\,T}{a^2\,z\,S}\right)^{3/2} \langle J^{-3/2} \rangle. \tag{20}$$

It is important to emphasize that the volume magnetization change of the inhomogeneous system has a $T^{3/2}$ dependence (like the homogeneous case) and also depends on the $-3/2$ moment of the distribution of exchange integrals $\langle J^{-3/2} \rangle$. This exponent is expected since 3 is related to the dimension of the system and 2 relates to the dynamics, i.e., comes from the dispersion relation (15).

2.2. Magnons within the homogeneous medium: the nonextensive framework

The dynamics of a system is given by its Hamiltonian $\mathcal{H}$ and the wavenumber k, defined by $\mathcal{H}$, is, consequently, related to the dynamics. On the other hand, the statistics of a system is given by an average over a great number of variables; and it lies, for instance, in the number of bosons n_k for each wavenumber k. This average over weighted states makes it possible to obtain the relation of microscopic physical properties and macroscopic thermodynamic quantities such as the volume magnetization variation. The nonextensive approach proposes a change of the statistics of the system, not of the dynamics. Thus, we assume an equivalent Hamiltonian (3), but homogeneous in this framework, i.e., the exchange integral can be taken out of the sum. The dispersion relation is therefore given by $\epsilon_k = a^2\,S\,\mathcal{J}\,k^2$, where $\mathcal{J}$ is the exchange integral of this homogeneous system. The volume magnetization in this nonextensive scenario can be written as [25]

$$\langle \Delta m \rangle_q = \frac{g\,\mu_{\rm B}}{2\,\pi} \int_0^\infty {\rm d}k\, k^2\, \langle\, n_k \rangle_{q,\mathcal{J}} \tag{21}$$

in which $n_k = b_k^+\,b_k$ is the boson number operator and $\langle \cdots \rangle_q$ is not the standard Planck distribution, but its q version, i.e., the generalized Plank distribution

$$\langle\, n_k \rangle_{q,\mathcal{J}} = \frac{{\rm Tr}\,\{n_k\,\rho^q\}}{{\rm Tr}\,\{\rho^q\}} = \frac{\sum_{n_k=0}^\infty n_k\,[1-(1-q)(\beta\,n_k\,\epsilon_k)]^{q/(1-q)}}{\sum_{n_k=0}^\infty [1-(1-q)(\beta\,n_k\,\epsilon_k)]^{q/(1-q)}}. \tag{22}$$

J. Stat. Mech. (2007) P08011

Using the dispersion relation described above and making (21) dimensionless, one gets

$$\langle \Delta\, m \rangle_q = \frac{g\,\mu_{\mathrm{B}}}{4\,\pi^2} \left(\frac{k_{\mathrm{B}}\,T}{a^2\,S\,\mathcal{J}}\right)^{3/2} \int_0^\infty \mathrm{d}x\, x^{1/2}\, f(x,q) \tag{23}$$

where

$$f(x,q) = \frac{\sum_{n_k=0}^{\infty} n_k\,[1-(1-q)(x\,n_k)]^{q/(1-q)}}{\sum_{n_k=0}^{\infty} [1-(1-q)(x\,n_k)]^{q/(1-q)}}. \tag{24}$$

Finally, the magnetization can be written as

$$\langle \Delta\, m \rangle_q = \frac{g\,\mu_{\mathrm{B}}}{4\,\pi^2} \left(\frac{k_{\mathrm{B}}\,T}{a^2\,S\,\mathcal{J}}\right)^{3/2} F(q) \tag{25}$$

where $F(q)$ is the integral which appears in equation (23). One can see that the magnetization in this scenario has the same $T^{3/2}$ behaviour as in (20). It is a consequence of neither the dynamics ($\epsilon_k \propto k^2$) nor the dimension ($d=3$) having changed. All the information about the homogeneity and/or inhomogeneity of the system is in the statistics and, consequently, in the coefficient of the magnetization change.

An analytical connection between the entropic parameter q and the volume magnetization change can be obtained at the limit $(q-1) \to 0$. At this limit, we can write (23) as

$$\langle n_k \rangle_{q,\mathcal{J}} = \frac{1/(\mathrm{e}^{q\,\beta\,\epsilon_k}-1) + (1/2)\,(\beta\,\epsilon_k)^2\,(q-1)\,(1+4\,\mathrm{e}^{q\,\beta\,\epsilon_k} + \mathrm{e}^{2\,q\,\beta\,\epsilon_k}/(\mathrm{e}^{q\,\beta\,\epsilon_k}-1)^3)}{1+(1/2)\,(\beta\,\epsilon_k)^2\,(q-1)\,(\mathrm{e}^{q\,\beta\,\epsilon_k}+1)/(\mathrm{e}^{q\,\beta\,\epsilon_k}-1)^2}. \tag{26}$$

Thus the volume magnetization change is now given by

$$\langle \Delta\, m \rangle_q = \frac{g\,\mu_{\mathrm{B}}}{2\,\pi^2} \int_0^\infty \mathrm{d}k\, k^2 \langle n_k \rangle_{q,\mathcal{J}} = \frac{g\,\mu_{\mathrm{B}}}{4\,\pi^2} \left(\frac{k_{\mathrm{B}}\,T}{a^2\,z\,S\,\mathcal{J}}\right)^{3/2} \left[\Gamma'_q + \frac{(q-1)}{2}\Gamma''_q\right] \tag{27}$$

in which Γ'_q and Γ''_q are dimensionless integrals

$$\begin{aligned}\Gamma'_q &= \int_0^\infty \frac{x^{1/2}\,\mathrm{d}x}{[\mathrm{e}^{q\,x}-1]\;[1+((q-1)/2)\,x^2\,([\mathrm{e}^{q\,x}+1]/[\mathrm{e}^{q\,x}-1]^2)]} \\ &= \frac{\sqrt{\pi}}{2}\,\zeta\left(\frac{3}{2}\right) - 5.2277\,(q-1)\end{aligned} \tag{28}$$

and

$$\begin{aligned}\Gamma''_q &= \int_0^\infty \frac{[1+4\,\mathrm{e}^{q\,x}+\mathrm{e}^{2\,q\,x}]\;x^{5/2}\,\mathrm{d}x}{[\mathrm{e}^{q\,x}-1]^3\;[1+((q-1)/2)\,x^2\,([\mathrm{e}^{q\,x}+1]/[\mathrm{e}^{q\,x}-1]^2)]} \\ &= 16.4154 - 68.6515\,(q-1).\end{aligned} \tag{29}$$

As it is an approximation for q close to 1, there is no necessity for terms higher than $(q-1)$, so the second term of Γ''_q can be neglected. Thus,

$$\langle \Delta\, m \rangle_q = \frac{g\,\mu_{\mathrm{B}}}{4\,\pi^2} \left(\frac{k_{\mathrm{B}}\,T}{a^2\,z\,S\,\mathcal{J}}\right)^{3/2} \left[\frac{\sqrt{\pi}}{2}\,\zeta\left(\frac{3}{2}\right) + 2.98\,(q-1)\right]. \tag{30}$$

One can see that, in this approximation, the magnetization is directly related to the entropic index and when $q \to 1$, it recovers the usual result (homogeneous case within BG statistics).

J. Stat. Mech. (2007) P08011

3. Mean field approximation and the critical temperature

Let us consider that the two systems discussed before have the same critical temperature, as already done in the literature [14]. Considering the Hamiltonian (3) for an inhomogeneous magnetic system within the mean field approximation, one may change the quantum operator $\mathbf{S}_{\mathbf{R+d}}$ to its thermal average $\langle \mathbf{S}_{\mathbf{R+d}} \rangle_T$. Thus, considering z first neighbours of an atom on the Rth site of the lattice, its Hamiltonian becomes

$$\mathcal{H}_{tr}^{R} = -\langle J \rangle \, z \, \mathbf{S}_{\mathbf{R}} \cdot \langle \mathbf{S}_{\mathbf{R+d}} \rangle_T \tag{31}$$

where in this approximation we can consider the exchange interaction between the spins as an average value $\langle J \rangle$. This is reasonable, because all of the spins, in the mean field approximation, interact with all other spins in the same way.

For the above Hamiltonian it is straightforward to obtain the critical temperature

$$T_{\mathrm{c}} = \frac{z \, S \, (S+1)}{3 \, k_{\mathrm{B}}} \langle J \rangle. \tag{32}$$

An analogous calculation can be carried out in the nonextensive scenario [26]. The generalized Brillouin function [2] gives us the critical temperature

$$T_{\mathrm{c}}^{(q)} = \frac{z \, S \, (S+1)}{3 \, k_{\mathrm{B}}} \, q \, \mathcal{J} \tag{33}$$

in which $\mathcal{J}$ is the exchange integral in this framework. The relation between these two temperatures is given by [14, 26]

$$T_{\mathrm{c}}^{(q)} = q \, T_{\mathrm{c}}^{(1)}. \tag{34}$$

Thus, using (32)–(34) one finds the relation between the two exchange integrals

$$\mathcal{J} = \langle J \rangle, \tag{35}$$

that is, the exchange integral in the nonextensive framework is equivalent to and average of the inhomogeneous one. This result is expected since, as already discussed above, we are not changing the dynamics of the system, only the statistical treatment which is used to calculate the thermodynamical properties of the system.

4. Equivalence of the two frameworks

Comparing the magnetization change per unit of volume in the inhomogeneous framework (21) with its analogue in the nonextensive scenario (25), one finds that

$$F(q) = \frac{\sqrt{\pi}}{2} \, \zeta\left(\frac{3}{2}\right) \frac{\langle J^{-3/2} \rangle}{\mathcal{J}^{-3/2}} = \frac{\sqrt{\pi}}{2} \, \zeta\left(\frac{3}{2}\right) \frac{\langle J^{-3/2} \rangle}{\langle J \rangle^{-3/2}}. \tag{36}$$

The above equation is a relation of the q parameter and moments of the exchange interaction distribution $f(J)$. Figure 1 presents the expression above numerically solved for $q \in [0.1, 1.9]$. This procedure comparing the magnetization has already been carried out [14], where similar results were found, with the authors inspired by superstatistics [19].

An analytical connection between the entropic parameter q and the specific moments of the exchange integral of the inhomogeneous magnetic media can be obtained using the

J. Stat. Mech. (2007) P08011

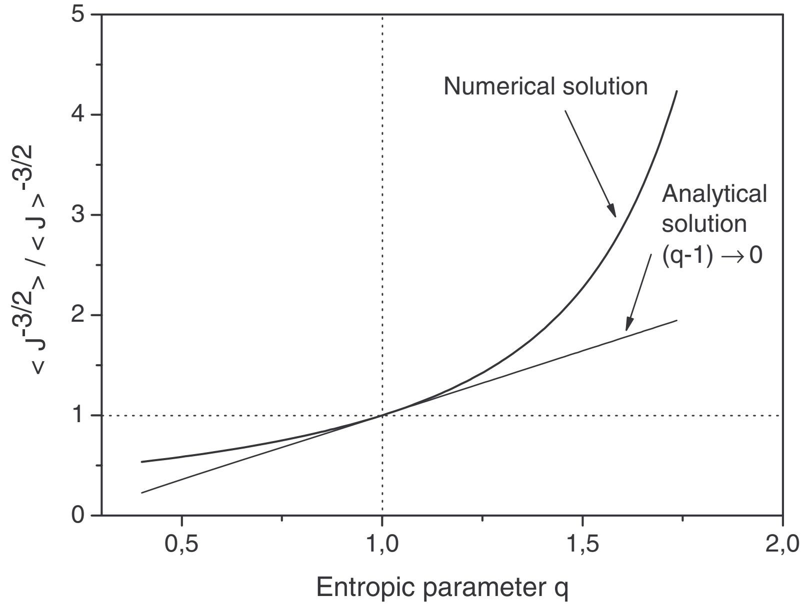

Figure 1. The entropic parameter q is connected to specific moments of the distribution of exchange integrals. This result is valid for any $f(J)$ and shows that the entropic parameter is connected to the physical properties of the system.

expression for the volume magnetization change in the limit $(q-1) \to 0$. Comparing (21) and (28) one gets

$$\frac{\sqrt{\pi}}{2}\zeta\left(\frac{3}{2}\right) + 2.98\,(q-1) = \frac{\sqrt{\pi}}{2}\zeta\left(\frac{3}{2}\right)\frac{\langle J^{-3/2}\rangle}{\langle J\rangle^{-3/2}} \tag{37}$$

or

$$(q-1) = 0.78\left[\frac{\langle J^{-3/2}\rangle}{\langle J\rangle^{-3/2}} - 1\right]. \tag{38}$$

The result above is also valid for any $f(J)$ and shows that the entropic parameter is connected to the physical properties of the system [2], [18]–[20].

5. Final remarks

Summarizing, in the present work we have shown that the q parameter can be seen as a measurement of the inhomogeneity of a magnetic system. This supports previous work [2, 3] in which, inspired in superstatistics [19], the authors related the entropic parameter q to the first and second moments of the distribution of magnetic moments of manganites:

$$q\,(2-q)^2 = \frac{\langle \mu^2\rangle}{\langle \mu\rangle^2} \tag{39}$$

and this was also experimentally verified. Thus, the present work supports the idea that changing the usual Boltzmann–Gibbs statistics to one that is able to describe power laws (Tsallis statistics), one can characterize systems that have special features like inhomogeneities; nonextensivity is therefore key for describing complex systems.

J. Stat. Mech. (2007) P08011

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J. Stat. Mech. (2007) P08011