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A study on composed nonextensive magnetic systems

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Abstract

We investigate the magnetic properties of a composed nonextensive system. The work is motivated by recent proposals that manganites are magnetically nonextensive objects, according to Tsallis statistics. We consider a two-parts composed system, $A-B$ (both spins $\frac{1}{2}$), and calculate self-consistently the partial magnetizations in the mean field approximation, M_A and M_B, for the cases the coupling between the subsystems is either ferro or anti-ferromagnetic. This involves the notion of partial trace in the nonextensive statistics. For temperatures below the magnetic ordering temperatures, and $q \neq 1$, we found strong disagreement between the M vs. T curves calculated from the total 4×4 Hilbert space, through ρ^q, when compared to the calculation made from the 2×2 subspaces, if we use the usual definition $\rho_{A(B)} \equiv \mathrm{Tr}_{B(A)}(\rho)$, and then elevates the matrices to the qth power, as adopted in other contexts in the literature of the nonextensive statistics. On another hand, full agreement is found if we take $\rho_{A(B),q} \equiv \mathrm{Tr}_{B(A)}(\rho^q)$, remaining q an implicit parameter.

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Keywords: Manganites; Non-extensive statistics; Partial trace

Manganese oxides, also named manganites, have recently been suggested as examples of systems where Tsallis nonextensivity is manifest [1–3]. In the context of mean field approximation, it was found a linear dependence between T_C and the entropic parameter

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q in La-based ferromagnetic manganites [1]; the anomalous behavior of the magnetic susceptibility was correctly described in the paramagnetic phase of $La_{2/3}Ca_{1/3}MnO_3$ [2] and the paramagnetic-ferromagnetic phase diagram of $La_{0.60}Y_{0.07}Ca_{0.33}MnO_3$ correctly reproduced using the nonextensive approach [3]. In this latter work it is analytically shown that the entropic parameter q is associated to the magnetic susceptibility of the material. Manganites exhibit the correct features for presenting nonextensivity: they are strong correlated long-range interaction systems [4], they present fractality [4] and they are magnetically inhomogeneous objects [5,6], with various properties dominated by intrinsic inhomogeneities [7,8]. It is therefore interesting to further investigate the magnetic properties of nonextensive systems. Moreover, the nonextensive statistics offers an alternative and simple approach to describe such an important class of magnetic materials, the manganites, which can be subject of experimental tests in a straightforward way, and therefore is a guide for first-principle models of magnetism.

In this paper we consider a composed $A-B$ spin $\frac{1}{2}$ system coupled either ferro or anti-ferromagnetically, in the mean field approximation. Here the concern is to investigate the calculation of marginal density matrices in the nonextensive context. This is important in a variety of situations: for classical information theory [9], for the study of criteria of separability in quantum mechanics [10,11], and for the foundations of the nonextensive statistics itself [12,13]. Although the concept of marginal density matrices appears in many works, no concrete example of application to magnetism has been presented to date. For this purpose magnetic systems are ideal because of their experimental connections to manganites.

We take a self-consistent mean field approximation, where the Hamiltonian is given by [14]:

$$\mathscr{H}_M = -2S_z^A B_A - 2S_z^B B_B \, , \tag{1}$$

where the mean field acting on each subsystem is:

$$B_A = B_0 + \lambda_A M_A + \lambda_{AB} M_B, \quad \text{and} \quad B_B = B_0 + \lambda_B M_B + \lambda_{AB} M_A \, . \tag{2}$$

B_0 is the external field. The intra-lattice couplings satisfy: $\lambda_A,\ \lambda_B > 0$, and the inter-lattices couplings satisfy : $\lambda_{AB} > 0$ for ferromagnetic and $\lambda_{AB} < 0$ for antiferromagnetic ordering.

Now, the subsystems magnetizations can be obtained in two different ways. Either we use the total density matrix, ρ^q:

$$M_A = 2\,\frac{\mathrm{Tr}(S_z^A \rho^q)}{\mathrm{Tr}(\rho^q)} \quad \text{and} \quad M_B = 2\,\frac{\mathrm{Tr}(S_z^B \rho^q)}{\mathrm{Tr}(\rho^q)} \, , \tag{3}$$

where $\rho^q = [1-(1-q)\beta' \mathscr{H}_M]^{q/1-q}/Z_q^q$, Z_q is the generalized partition function, and $\beta' = \beta/(1/\mathrm{Tr}(\rho^q) + (1-q)\beta U_q)$ or we use marginal matrices, obtained from partial tracing the total density matrix.

Before starting the calculations, it is interesting to note that the above distribution of probabilities is obtained from the maximization of the (normalized) nonextensive entropy (Tsallis entropy) [15]:

$$S_q = \frac{1-\mathrm{Tr}(\rho^q)}{(q-1)\mathrm{Tr}\rho^q} \tag{4}$$

subject to the norm and energy constraints:

$$\mathrm{Tr}(\rho)=1, \quad U_q=\frac{\mathrm{Tr}(\mathscr{H}\rho^q)}{\mathrm{Tr}(\rho^q)} . \tag{5}$$

So we have the averaged value

$$\mathcal{O}_q=\frac{\mathrm{Tr}(\mathcal{O}\rho^q)}{\mathrm{Tr}(\rho^q)} . \tag{6}$$

Notice that the averaged value in the nonextensive formalism of an observable O is different from the usual one, and can be formally related to the usual form by using the escort distributions, i.e., $P=\rho^q/\mathrm{Tr}(\rho^q)$, with the inverse relation being given by $\rho=P^{1/q}/\mathrm{Tr}(P^{1/q})$. In particular, the nonextensive statistical mechanics has been applied in several situations such as anomalous diffusion [16], evolution of stellar self-gravitating systems away from thermal equilibrium [17], anomalous relaxation through electron–phonon interaction [18], ferrofluid-like systems [19], dynamic systems [20] and to study the microscopic dynamics of the metastable quasi-stationary states in the Hamiltonian mean field model [21].

Eqs. (2) and (3) must be solved self-consistently. In the case of a two spin $\frac{1}{2}$ system, the calculation involves summing in either a 4×4 Hilbert space or two 2×2 subspaces. Of course, since the magnetization is a thermodynamic observable, both approaches must yield the same result. Our goal is to compare two ways of partial tracing, and show that full agreement occurs only for one of them. In the first one, which we will call method I, the marginal densities are obtained from:

$$\rho_A=\mathrm{Tr}_B(\rho) \quad \text{and} \quad \rho_B=\mathrm{Tr}_A(\rho) \tag{7}$$

after convergence is achieved, and then subsequently powered to q; to obtain M_A and M_B, we simply replace the 4×4 matrix ρ^q in Eq. (3) by the 2×2 matrices ρ_A^q and ρ_B^q. This is the approach used, for instance, in Refs. [9,10] in the context of separability of quantum systems.

In method II, we set $\rho'\equiv\rho^q$ and partial trace ρ', remaining the entropic index implicit:

$$\rho_{A,q}=\mathrm{Tr}_B(\rho^q) \quad \text{and} \quad \rho_{B,q}=\mathrm{Tr}_A(\rho^q) . \tag{8}$$

It is shown below that only method II reaches full agreement with the calculation made with the total density matrix. Therefore, at least in the context of nonextensive magnetism, the relevant statistical quantity seems to be ρ', instead of ρ.

Fig. 1(a) exhibits M_A vs. T curves obtained self-consistently with method I, for various values of q, and $B_0=0$. Full circles are calculations made with the marginal density matrix, ρ_A^q, and continuous lines are calculations using the complete 4×4 density matrix. The disagreement for q below 0.9 is evident. Fig. 1(b) shows the same calculations made with method II. We see that in this case there is plain agreement for the full range of temperature and all values of q. Figs. 2(a) and (b) show the corresponding curves for the anti-ferromagnetic case. We see that for $B_0=0$ the total magnetization is always equal to zero in both cases, but the disagreement in method I for $q<0.9$ is again evident.

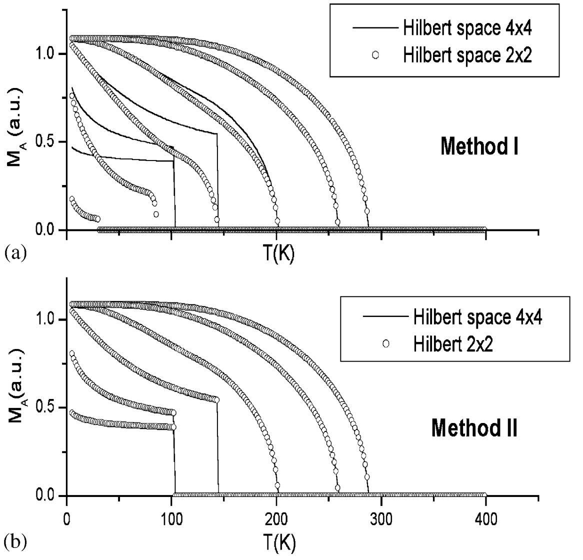

Fig. 1. (a) Comparison of M vs. T curves calculated with method I (see text) for sublattice A in the ferromagnetic case ($\lambda_{AB} > 0$). Continuous lines are calculations from the full 4×4 density matrices, and dots are calculations with the reduced ρ_A^q. Sublattice B shows the same behavior. The values of q from left to right curves are $q = 0.1, 0.3, 0.5, 0.7, 0.9, 1.0$. (b) Same curves calculated with method II.

This paper focused in the concept of partial tracing and marginal densities of composed systems in the nonextensive statistics. This is important in a variety of situations, and manganites offer an access door to experimentally testing these ideas. From measuring M vs. T curves for various values of the external field, B_0, the specific heat can be derived [22,23]. In more realistic models of manganites, different ionic species and the effects of crystal-field, including the Jean–Teller effect must be taken into account [4,24,25].

On the nonextensive statistics side, it is very important to come up with a clear concept of partial tracing. The famous formula of the pseudo-additivity for the entropies of nonextensive systems [12]

$$S_q(A+B) = S_q(A) + S_q(B) + (1-q)S_q(A)S_q(B)$$

relies on the assumption that for statistically independent systems, the relation $\rho^q = \rho_A^q \otimes \rho_B^q$ holds, and therefore it is important to know how to obtain ρ_A and ρ_B for composed systems. The quantities $\rho_{A,q}$ and $\rho_{B,q}$ used in this paper to calculate the sublattice magnetizations cannot be connected in a simple way to the definition adopted in other works, for instance in Ref. [10]. Very recent developments [26] show that nonextensive entropies can become additive for particular values of q. Since the magnetization of a sample must be proportional to the number of magnetic moments (a natural consequence of the additivity of entropies), there may be important connections

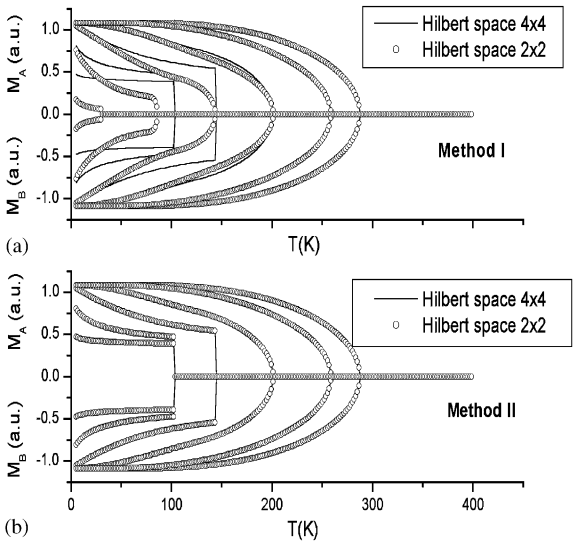

Fig. 2. (a) Comparison of M vs. T curves calculated with method I (see text) for sublattices A and B in the antiferromagnetic case ($\lambda_{AB} < 0$). Continuous lines are calculations from the full 4×4 density matrices, and dots are calculations with the reduced matrices ρ_A^q and ρ_B^q. The values of q from left to right curves are $q = 0.1, 0.3, 0.5, 0.7, 0.9, 1.0$. (b) Same curves calculated with method II.

between such particular values of q and the physical parameters of the system, such as T_C, as suggested in the present paper and in Ref. [1].

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References

[1] M.S. Reis, J.C.C. Freitas, M.T.D. Orlando, E.K. Lenzi, I.S. Oliveira, Europhys. Lett. 58 (1) (2002) 42.
[2] M.S. Reis, J.P. Araujo, V.S. Amaral, E.K. Lenzi, I.S. Oliveira, Phys. Rev. B 66 (2002) 134417.
[3] M.S. Reis, V.S. Amaral, J.P. Araujo, I.S. Oliveira, Phys. Rev. B 68 (2003) 014404.
[4] E. Dagotto, T. Hotta, A. Moreo, Phys. Rep. 344 (2001) 1.
[5] R. Caciuffo, D. Rinaldi, G. Barucca, J. Mira. J. Rivas, M.A. Senaris-Rodriguez, P.G. Radaelli, D. Fiorani, J.B. Goodenough, Phys. Rev. B 59 (1999) 1068.
[6] D.N.H. Nam, K. Jonason, P. Nordblad, N.V. Khiem, N.X. Phuc, Phys. Rev. B 59 (1999) 4189.
[7] M.S. Reis, V.S. Amaral, P.B. Tavares, A.M. Gomes, A.Y. Takeuchi, A.P. Guimares, I.S. Oliveira, P. Panissod, cond-mat/0211143, unpublished.
[8] Y. Tokura, Y. Tomioka, J. Magn. Magn. Mater. 200(1–3) (1999) 1.
[9] S. Abe, A.K. Rajagopal, Physica A 289 (2001) 157.
[10] C. Tsallis, S. Loyd, M. Baranger, Phys. Rev. A 63 (2001) 0142104.
[11] A.K. Rajagopal, R.W. Rendell, Phys. Rev. A 66 (2002) 022104.
[12] C. Tsallis, Braz. J. Phys. 29 (1999) 1.
[13] C. Tsallis, in: S. Abe, Y. Okamoto (Eds.), Non-extensive Statistical Mechanics and its applications, Lecture Notes in Physics Vol. 560, Springer, Berlin, 2001.

[14] A.P. Guimares, Magnetism and Magnetic Resonance in Solids, Wiley Inter Sciences, New York, 1998.
[15] S. Abe, A.K. Rajagopal, Phys. Rev. Lett. 83 (1999) 1711.
[16] A.R. Plastino, A. Plastino, Physica A 222 (1995) 347;
C. Tsallis, D.J. Bukman, Phys. Rev. E 54 (1996) R2197;
P.H. Chavanis, C. Sire, Phys. Rev. E 69 (2004) 016116;
P.H. Chavanis, Physica A 89 (2004) 332.
[17] A. Taruya, M. Sakagami, Phys. Rev. Lett. 90 (2003) 181101.
[18] I. Koponen, Phys. Rev. E 55 (1997) 7759.
[19] P. Jund, S.G. Kim, C. Tsallis, Phys. Rev. B 52 (1995) 50.
[20] C. Beck, F. Schlgl, Thermodynamic of Chaotic Systems, Cambridge University Press, Cambridge, 1993.
[21] A. Pluchino, V. Latora, A. Rapisarda, Metastable states, anomalous distributions and correlations in the HMF model, cond-mat/0303081.
[22] A.M. Aliev, Sh.B. Abdulvagidov, A.B. Batdalov, I.K. Kamilov, O.Yu. Gorbenko, V.A. Amelichev, A.R. Kaul, A.I. Kurbakov, V.A. Trunov, Phys. Sol. Stat. 45 (1) (2003) 130.
[23] J. Lopez, O.F. de Lima, J. Appl. Phys. 94 (7) (2003) 4395.
[24] Zhao-hua Cheng, Zhi-hong Wang, Nai-li Di, Zhi-qi Kou, Guang-jun Wang, Rui-wei Li, Yi Lu, Qing-an Li, Bao-gen Shen, Appl. Phys. Lett. 83(8) (2003) 1587.
[25] S.M. Dunaevski, Phys. Sol. Stat. 43 (12) (2001) 2257.
[26] C. Tsallis, in: H.L. Swinney, C. Tsallis (Eds.), Anomalous distributions, nonlinear dynamics and nonextensivity, Physica D 193 (2004) 3.