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NEW CONSIDERATION ON COMPOSED NONEXTENSIVE MAGNETIC SYSTEMS

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In this paper, a composed A + B magnetic system, with spins $J_{\rm A} = 2$ and $J_{\rm B} = 3/2$, is considered within the mean-field approximation, in the framework of Tsallis nonextensive statistics. Our motivation is twofold: (1) to approach the existing experimental data of manganese oxides (manganites), where Mn^{3+} and Mn^{4+} form two magnetic sublattices, and (2) to investigate the structure of nonextensive density matrices of composed systems. By imposing that thermodynamic quantities, such as the magnetization of sublattices A and B, must be invariant whether the calculation is taken over the total Hilbert space or over partial subspaces, we found that the expression for the nonextensive entropy must be adapted. Our argument is supported by the calculation of sublattice magnetizations $M_{\rm A}$ and $M_{\rm B}$, internal energy, $U_{\rm A}$ and $U_{\rm B}$ and magnetic specific heat, $C_{\rm A}$ and $C_{\rm B}$. It is shown that only with the modified entropy, the two methods of calculation agree to each other. Internal energy and magnetization are additive, but no clear relationship was found between $S_{\rm A}$, $S_{\rm B}$ and the total entropy $S_{\rm A+B}$ for $q \neq 1$. It is shown that the reason for the failure of the standard way of calculation is the assumption of statistical independence between the two subsystems, which however does not affect the density matrix in the full Hilbert space.

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1. Introduction

Recently, Reis et al. [1 − 3] have provided experimental evidences that the magnetic properties of manganese oxides, or simply manganites, must be interpreted within the framework of Tsallis non-extensive statistics [4, 5]. This proposal should interest both, the magnetic and the statistical physics communities, for at least two reasons: (1) up to date no first-principle model is known to account for the whole complexity of the physical properties of manganites. Therefore, phenomenological tools to treat these materials should be welcome; (2) samples of manganites are simple to be made, and even sophisticated high purity single crystal samples are nowadays available [6]. Therefore, from one hand manganites are an easy way to test the consequences of nonextensive statistics and, from another, nonextensive statistics is a parametrical tool to treat manganites. One of the greatest challenges of the theoretical nonextensive framework is to find relationships between the entropic parameter q and the dynamical variables of a system. In Ref. [3] it is analytically shown that q relates to the magnetic susceptibility of the material. Finally, one must mention that manganites present many of the correct ingredients for nonextensivity: they are fractal [6], they are inhomogeneous [7, 8] and they exhibit long-range interaction [6].

In a previous publication [9] we investigated the magnetic properties of a nonextensive composed system of two spins 1/2 within the mean-field approximation. It was shown that in order the sublattices magnetization, calculated from the full Hilbert space, to agree with the same quantity calculated from the subspaces, the respective partial traces should be performed over the quantity ρ^q instead of ρ. This conflicts with the standard approach, and raises important questions concerning the structure of nonextensive density matrix space, particularly the notion of statistical independence. Besides, ρ^q cannot be interpreted as a true density matrix, since it is not normalized. In the present paper, we carried the analysis further and show that with an appropriate modification in the definition of the nonextensive entropy, it is possible to keep the usual interpretation of partial tracing, at the same time making the two methods of calculation agree to each other. Such a modification does not affect the usual formalism in any fashion, whenever full Hilbert space is under consideration. The starting point is the simple remark that thermodynamic observables of a composed system must not depend on the dimension of Hilbert spaces. Therefore, we impose the following guiding principle for a composed A + B system,

$$O_f = O_p\,, \tag{1}$$

where O is a thermodynamic quantity of either subsystem, corresponding to a quantum mechanical observable $\widehat{O}$. The subscripts f and p stand for *full* and *partial* Hilbert spaces, respectively.

2. Model

Similarly to what was done in Ref. [10], we propose that nonextensive entropy must be defined as

$$S_q = -k_B \frac{\mathrm{Tr}\big[\rho^q \ln(\rho^q)\big]}{\mathrm{Tr}(\rho^q)}\,, \tag{2}$$

and the q-logarithm [4, 5]:

$$\ln_q(\rho) = \frac{\rho^{1-q} - I}{1-q}\,, \tag{3}$$

where I is the identity matrix in the full Hilbert space. From (2) and (3), we obtain the normalized form of the nonextensive entropy [11]

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

Maximization of S_q in Eq. (4), subject to the norm and energy constraints

$$\mathrm{Tr}(\rho^q) = 1 \qquad \text{and} \qquad U_q = \frac{\mathrm{Tr}(\rho^q H)}{\mathrm{Tr}(\rho^q)}\,, \tag{5}$$

leads to the well known probability distribution

$$\rho = \frac{\{1 - (1-q)\beta^* H\}^{1/(1-q)}}{Z_q}\,, \tag{6}$$

where Z_q is the generalized partition function

$$Z_q = \mathrm{Tr}\{1 - (1-q)\beta^* H\}^{1/(1-q)} \tag{7}$$

and

$$\beta^* = \frac{1}{k_B T}\,, \tag{8}$$

with T, the physical temperature and k_B the Boltzmann constant. According to this, if ρ describes a composed A + B system, each subsystem entropy should be given, in the full Hilbert space, by

$$S_\mathrm{A} = -k_B \frac{\mathrm{Tr}\big[\rho^q \ln(\rho'_\mathrm{A})\big]}{\mathrm{Tr}(\rho^q)} \qquad \text{and} \qquad S_\mathrm{B} = -k_B \frac{\mathrm{Tr}\big[\rho^q \ln(\rho'_\mathrm{B})\big]}{\mathrm{Tr}(\rho^q)}\,, \tag{9}$$

where:

$$\rho'_\mathrm{A} = \rho_A \otimes I_\mathrm{B} \qquad \text{and} \qquad \rho'_\mathrm{B} = I_\mathrm{A} \otimes \rho_\mathrm{B}\,, \tag{10}$$

where I_A and I_B are the identity matrices in the respective Hilbert subspaces, and $\rho_\mathrm{A} = \mathrm{Tr}_\mathrm{B}(\rho)$ and $\rho_\mathrm{A} = \mathrm{Tr}_\mathrm{A}(\rho)$.

Upon the assumption of statistical independence

$$\rho^q_{\rm A+B} = \rho^q_{\rm A} \otimes \rho^q_{\rm B}\,, \tag{11}$$

the standard formulae for the entropies in the subspaces are obtained. We denominated this the method I

$$S_{\rm A} = -k_B \frac{1-{\rm Tr}(\rho^q_{\rm A})}{(q-1){\rm Tr}(\rho^q_{\rm A})} \qquad \text{and} \qquad S_{\rm B} = -k_B \frac{1-{\rm Tr}(\rho^q_{\rm B})}{(q-1){\rm Tr}(\rho^q_{\rm B})} \tag{12}$$

which relates to the total entropy, $S_{\rm A+B}$, through the formula

$$S_{\rm A+B} = \frac{S_{\rm A}}{{\rm Tr}(\rho^q_{\rm B})} + \frac{S_{\rm B}}{{\rm Tr}(\rho^q_{\rm A})} + (1-q)S_{\rm A}S_{\rm B}\,. \tag{13}$$

However, in order to preserve the traditional and well established notions of partial traces and expected values, we propose that the correct way to calculate the subsystems entropy (in the subspaces A and B) must include weight factors $E_{\rm A}$ and $E_{\rm B}$. We call this procedure the method II,

$$S_{\rm A} = -k_B \frac{{\rm Tr}\big[E_{\rm A}\ln(\rho_{\rm A})\big]}{{\rm Tr}(E_{\rm A})} \qquad \text{and} \qquad S_{\rm B} = -k_B \frac{{\rm Tr}\big[E_{\rm B}\ln(\rho_{\rm B})\big]}{{\rm Tr}(E_{\rm B})}\,, \tag{14}$$

where

$$E_{\rm A} = {\rm Tr}_B(\rho^q) \qquad \text{and} \qquad E_{\rm B} = {\rm Tr}_A(\rho^q)\,. \tag{15}$$

The E factors can also be included in the definition of the non-normalized form of Tsallis entropy. This will affect only the expression for the energy parameter β^* [2].

We will now exemplify the above considerations with the case of a system composed by two magnetically coupled sublattices, A and B, with spins $J_{\rm A} = 2$ and $J_{\rm B} = 3/2$. These are the spins of free ion Mn^{3+} and Mn^{4+}, respectively. In the mean-field approximation, the Hamiltonian is given by [12]

$$H_{\rm M} = H_{\rm A} + H_{\rm B}\,, \tag{16}$$

with

$$H_{\rm A} = -g_{\rm A} J^z_{\rm A} B_{\rm A} \qquad \text{and} \qquad H_{\rm B} = -g_{\rm B} J^z_{\rm B} B_{\rm B}\,, \tag{17}$$

where the effective field acting one each subsystem is

$$B_{\rm A} = B_0 + \lambda_{\rm A} M_{\rm A} + \lambda_{\rm AB} M_{\rm B} \qquad \text{and} \qquad B_{\rm B} = B_0 + \lambda_{\rm B} M_{\rm B} + \lambda_{\rm AB} M_{\rm A}\,, \tag{18}$$

where B_0 is the external field and $g_{\rm A} = 2/3$ and $g_{\rm B} = 4/5$. The intralattice couplings satisfy $\lambda_{\rm A}, \lambda_{\rm B} > 0$, and the interlattices couplings satisfy $\lambda_{\rm AB} > 0$ for ferromagnetic and $\lambda_{\rm AB} < 0$ for antiferromagnetic ordering [13].

In the present case, the dimension of the full Hilbert space is 20×20, and the Hilbert subspaces of the subsystems are 5×5 ($J^{\rm A} = 2$) and 4×4 ($J^{\rm B} = 3/2$) dimensional. In the usual formalism, the method I, we have that the sublattices magnetizations are given by

$$M_{\rm A} = g_{\rm A}\frac{{\rm Tr}(\rho_{\rm A}^q J_{\rm A}^z)}{{\rm Tr}(\rho_{\rm A}^q)} \qquad \text{and} \qquad M_{\rm B} = g_{\rm B}\frac{{\rm Tr}(\rho_{\rm B}^q J_{\rm B}^z)}{{\rm Tr}(\rho_{\rm B}^q)}\,, \tag{19}$$

where

$$\rho_{\rm A(B)}^q = \left\{{\rm Tr}(\rho_{\rm B(A)}\right\}^q\,, \tag{20}$$

whereas according to our proposal (the method II), they are given by

$$M_{\rm A} = g_{\rm A}\frac{{\rm Tr}(E_{\rm A} J_{\rm A}^z)}{{\rm Tr}(E_{\rm A})} \qquad \text{and} \qquad M_{\rm B} = g_{\rm B}\frac{{\rm Tr}(E_{\rm B} J_{\rm B}^z)}{{\rm Tr}(E_{\rm B})}\,. \tag{21}$$

In the full Hilbert space we obviously have

$$M_{\rm A(B)} = g_{\rm A(B)}\frac{{\rm Tr}(\rho^q J_{\rm A(B)}^z)}{{\rm Tr}(\rho^q)}\,. \tag{22}$$

Similarly, the contributions of each sublattice to the internal energy are

$$U_{\rm A} = \frac{{\rm Tr}(E_{\rm A} H_{\rm A})}{{\rm Tr}(E_{\rm A})} \qquad \text{and} \qquad U_{\rm B} = \frac{{\rm Tr}(E_{\rm B} H_{\rm B})}{{\rm Tr}(E_{\rm B})}\,, \tag{23}$$

and to the specific heat [14]

$$C_{\rm A} = T\left\{\frac{\partial S_{\rm A}}{\partial T}\right\}_{B_0} \qquad \text{and} \qquad C_{\rm B} = T\left\{\frac{\partial S_{\rm B}}{\partial T}\right\}_{B_0}. \tag{24}$$

Notice that, for $q \neq 1$, the nonadditivity of the entropies leads to nonadditivity of the specific heat. The above quantities were calculated self-consistently using the two approaches, the standard one and our proposal.

3. Computational simulations

Figure 1 shows the comparison between the temperature dependence of the magnetization of sublattices A and B, calculated in the full Hilbert space with the method I, Eq. (21), and the method II, Eq. (23). The two methods are equivalents only for the values of q close to 1. Therefore, the Boltzmann-Gibbs statistics does not present difficulties at different Hilbert spaces.

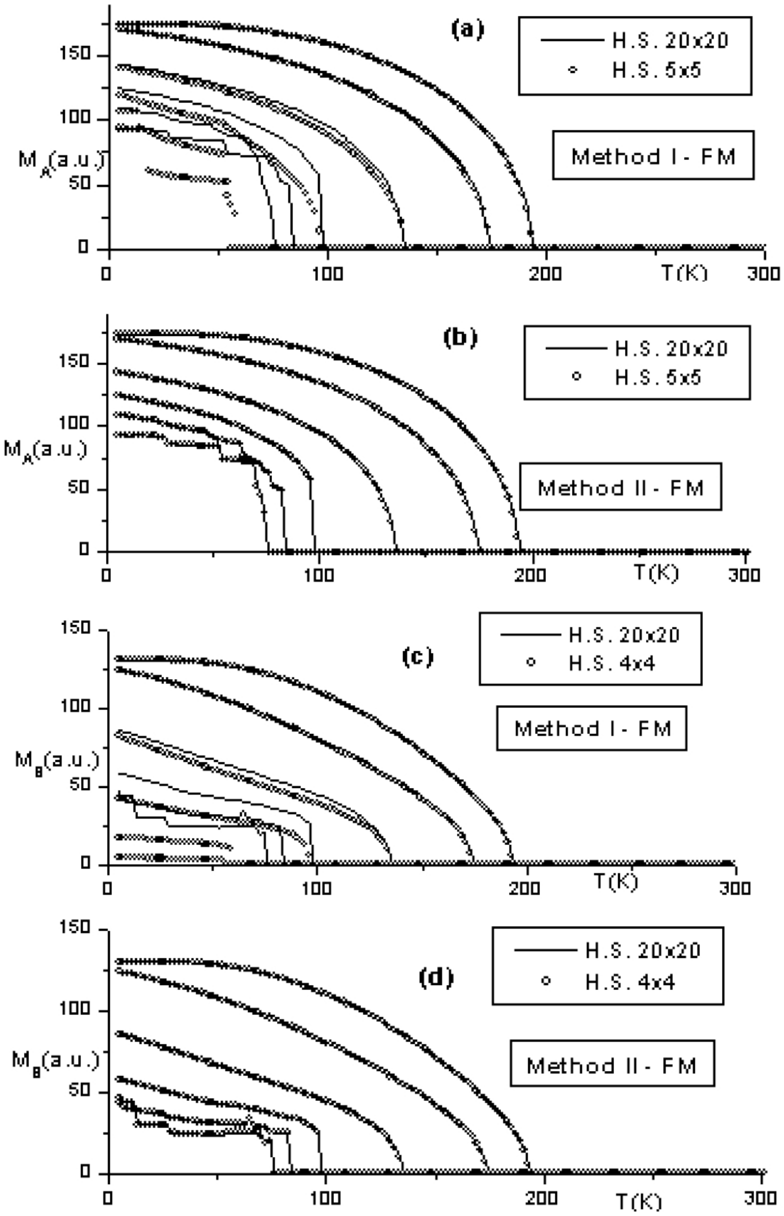

Fig. 1. Magnetizations of sublattices A *and* B *of a ferromagnetically coupled system. Continuous line is the calculation made in the full Hilbert space, and symbols are the results of calculation in subspaces using either method I or II. Notice that the method II reaches plain agreement with the calculation in full Hilbert space. The values of q, from bottom up, are 0.1, 0.3, 0.5, 0.7, 0.9 and 1.0. This remark is also valid for Fig. 2 and Fig. 3.*

Figure 2 shows similar results for the internal energies U_A and U_B. Moreover, only the method II reaches plain agreement with the calculation in full Hilbert space. The values of q, from the top down, are 0.1, 0.3, 0.5, 0.7, 0.9 and 1.0.

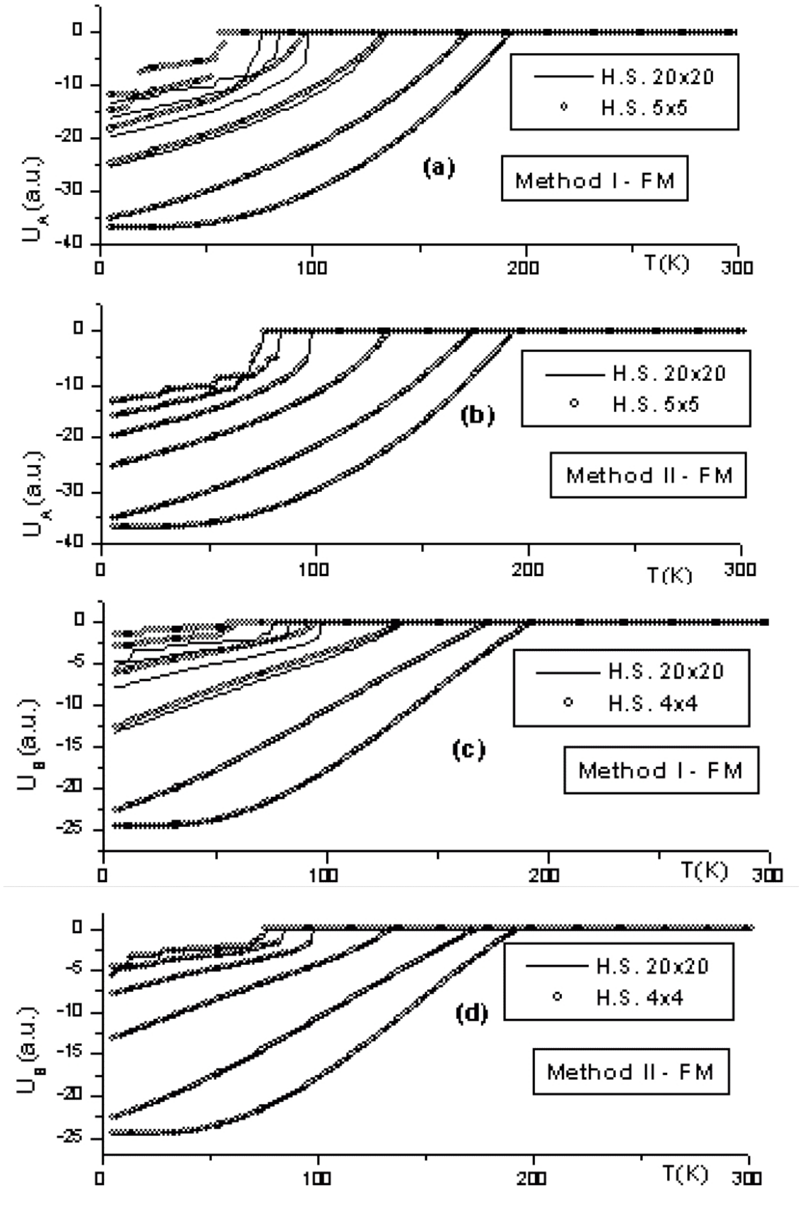

Fig. 2. Internal energies of sublattices A *and* B *of a ferromagnetically-coupled system. Continuous line is the calculation made in the full Hilbert space, and symbols are the results of calculation in subspaces using either method I or II.*

Figure 3 compares the contributions to the specific heat. The values of q, from the bottom up, are 0.1, 0.3, 0.5, 0.7, 0.9 and 1.0.

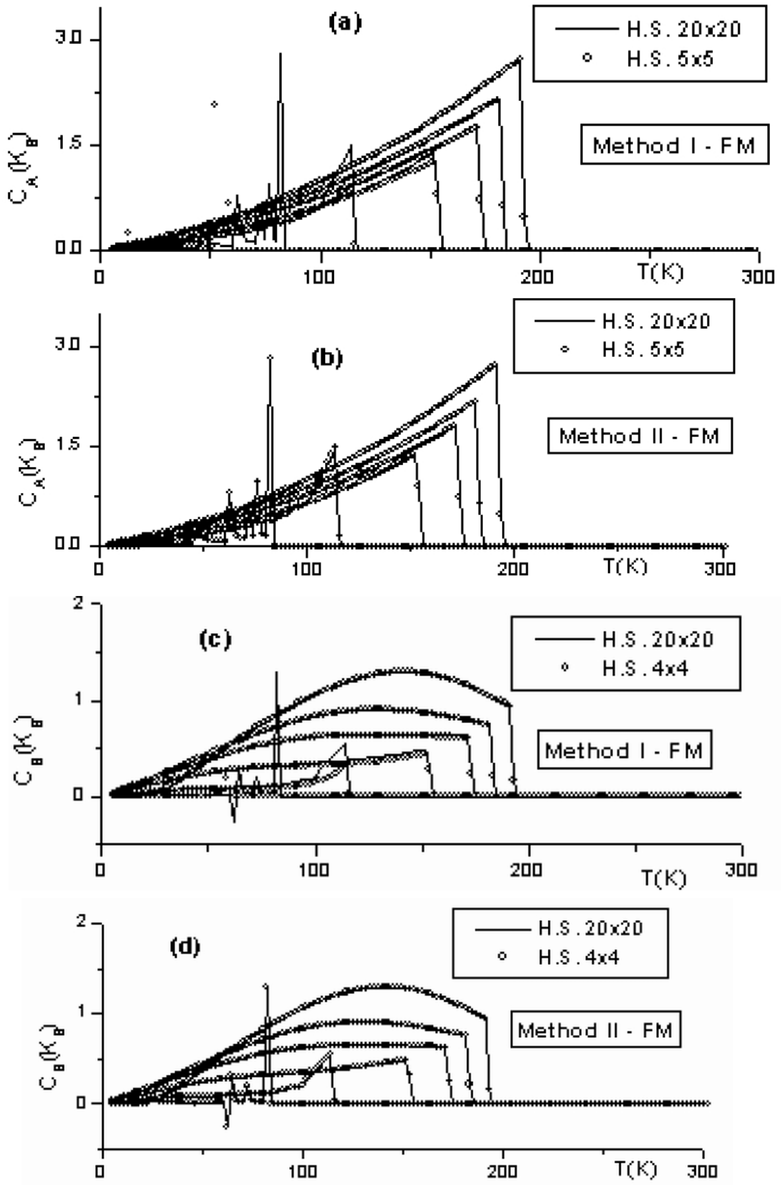

Fig. 3. Contribution to the magnetic specific heat from sublattices A *and* B *of a ferromagnetically-coupled system. Continuous line is the calculation made in the full Hilbert space, and symbols are the results of calculation in subspaces using either method I or II. The latter method II is correct.*

Figure 4 shows that nonextensive magnetizations and internal energy become additive only in the method II. Calculations were made for q values 0.3 and 0.7.

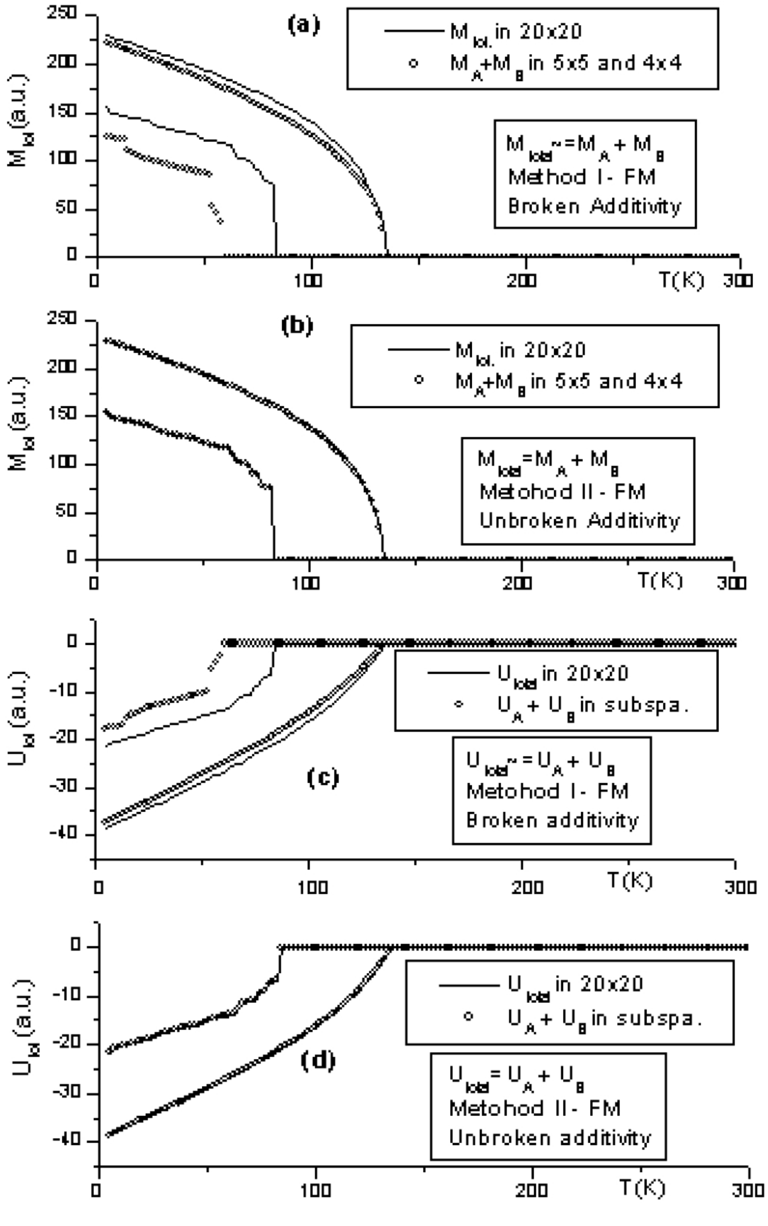

Fig. 4. The additivity in the nonextensive formalism occurs only in the method II of calculation. This is a desired property for a magnetic system, since it preserves the total number of spins.

4. Conclusions

In conclusion, one could not derive an analytical expression relating $S_{\rm A}$ and $S_{\rm B}$ to $S_{\rm A+B}$. The reason for the failure of the standard method of calculation (the method I), Eqs. (21) (and similar expressions for other quantities) is that it is valid only for statistically independent systems, a notion which is still not clear in the context of nonextensive statistics, and of course does not apply to the case of coupled magnetic systems. On the other hand, the standard expressions can be derived from the expressions (23) and (25), which can then be considered a generalization of the first ones. These observations apply to the entropy, as well. Therefore, we conclude that Eqs. (14) must replace the usual expressions, Eqs. (12) for the entropy of nonextensive composed systems. The analysis of the nonextensive entropy of composed systems and their applications in systems such as alloys, glasses and magnetoresistive materials [14−16], is an important aspect to the formalism of nonextensive statistics, but which has not been enough developed. On one hand, the possibility of making an experimental connection to manganites opens up the possibility of laboratorial tests [2] of the formalism, and on another hand offers to the magnetism community a convenient parametric tool to interpret and classify the magnetic behaviour of manganites.

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NOVA RAZMATRANJA MALIH SLOŽENIH MAGNETSKIH SUSTAVA

Razmatramo magnetski sustav složen od sastavnica A i B sa spinovima $J_{\rm A} = 2$ i $J_{\rm B} = 3/2$ u približenju srednjeg polja i Tsallisove nesveobuhvatne statistike. Dva su povoda: (1) opisati poznate mjerne podatke za manganove okside (manganite), u kojima $\rm Mn^{3+}$ i $\rm Mn^{4+}$ tvore dvije magnetske podrešetke, i (2) istražiti strukturu nesveobuhvatne matrice gustoće složenih sustava. Postavljajući da termodinamičke veličine, kao magnetizacija podrešetaka A i B, moraju biti invarijantne kako za račun u cijelom Hilbertovom prostoru, tako i u pojedinim podrešetkama, nalazimo da se izraz za nesveobuhvatnu entropiju mora primijeniti. Naša tvrdnja se zasniva na računu magnetizacije podrešetaka $M_{\rm A}$ i $M_{\rm B}$, unutarnje energije $U_{\rm A}$ i $U_{\rm B}$, i magnetske specifične topline, $C_{\rm A}$ i $C_{\rm B}$. Pokazuje se da su s izmijenjenom entropijom obje metode u skladu. Unutarnja energija i magnetizacija se pribrajaju, ali između $S_{\rm A}$, $S_{\rm B}$ i ukupne entropije $S_{\rm A+B}$ nismo našli jednostavan odnos za $q \neq 1$. Pokazuje se da je pretpostavka o neovisnosti dvaju podsustava razlog što uobičajen način računanja entropije nije dobar, što ne utječe na račun matrice gustoće u cijelom Hibertovom prostoru.