



CBPF-CENTRO BRASILEIRO DE PESQUISAS FÍSICAS

Notas de Física

CBPF-NF-028/94 July 1994

Infinite-Range Ising Ferromagnet: Thermodynamic Limit Within Generalized Statistical Mechanics

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Abstract

We first discuss, for a variety of similar systems, the physical need for departure from Boltzmann-Gibbs statistical mechanics and thermodynamics. Then, we numerically discuss the infinite-range spin-1/2 Ising ferromagnet within the recently generalized statistical mechanics (canonical ensemble). Through the specific heat, we exhibit (for the first time, as far as we know, for an interacting system) that the thermodynamic limit is well defined.

Keywords: Generalized Entropy; Nonextensive Thermodynamics; Ising Ferromagnet;

Long-Range Interactions.

PACS Numbers: 02.50.+s, 05.50.+q, 05.70.-a, 05.90.+m.

1. Introduction

During recent years, nonextensive formalisms are quickly growing in Physics. We mainly refer here to Quantum-Group-like approaches [1-13], and to the Generalized Statistical Mechanics and Thermodynamics [14-30] to which the present paper is dedicated.

The physical motivations for such attempts concern a great variety of systems: black holes and superstrings [31], d = 3 self-gravitating astrophysical objects [32], Lévy random walks [33], vortex problem [34], nonlocalizability of the photon [35], dark matter [11], stability of granular matter such as a sandpile, and many others. In all the cases, spatial-temporal long-range microscopic interactions (i.e., either long-range space interactions or long-range memory, or both) seem to be involved, in one way or another [24,25]; one such situation occurs whenever the relevant space-time of the problem is fractal (or multifractal), since the scale invariance acts as a kind of long-range transport of information. Some of the situations above mentioned are discussed in more detail in Section 2. Let us now briefly recall what the Generalized Statistical Mechanics and Thermodynamics is about.

One of us [14] proposed a generalized expression for the entropy, namely

$$S_q = k \frac{1 - \sum_{s=1}^W p_s^q}{q - 1} \qquad (q \in \Re) \qquad , \tag{1}$$

where q characterizes the statistics, k is a conventional positive constant, and $\{p_s\}$ are the probabilities associated with the W microscopic configurations that might occur in the system. Eq. (1) recovers, for $q \to 1$, the well-known Boltzmann-Gibbs-Shannon expression, $S_1 = -k_B \sum_s p_s \ln p_s$. S_q is nonnegative, extremal for equiprobability, i.e., for $p_s = 1/W$, $\forall s$ (microcanonical ensemble; the entropy is given by $S_q = k(W^{1-q}-1)/(1-q)$, which generalizes $S_1 = k_B \ln W$), expansible for q > 0, concave (convex) for all $\{p_s\}$ if q > 0 (q < 0), a fact which garantees thermodynamic stability for the system. S_q satisfies the H-theorem [16], i.e., $dS_q/dt \geq 0$ (≤ 0) if q > 0 (q < 0), and is pseudoadditive for two independent systems Σ and Σ' (i.e., if $\hat{\rho}_{\Sigma \cup \Sigma'} = \hat{\rho}_{\Sigma} \otimes \hat{\rho}_{\Sigma'}$, where $\hat{\rho}$ denotes the density operator, whose eigenvalues are the $\{p_s\}$; $\hat{\rho}_{\Sigma \cup \Sigma'}$ acts on the tensor product of the Hilbert

spaces respectively associated with Σ and Σ'); in other words, it satisfies

$$\frac{S_q^{\Sigma \cup \Sigma'}}{k} = \frac{S_q^{\Sigma}}{k} + \frac{S_q^{\Sigma'}}{k} + (1 - q) \frac{S_q^{\Sigma}}{k} \frac{S_q^{\Sigma'}}{k} \qquad (2)$$

Consequently, unless q = 1, S_q is generically nonextensive (nonadditive).

If the system is in thermal equilibrium with a thermostat at temperature $T \equiv 1/\beta k$ we must optimize S_q under the constraints $\text{Tr}\hat{\rho} = 1$ and $\text{Tr}(\hat{\rho}^q\hat{\mathcal{H}}) \equiv \langle \hat{\mathcal{H}} \rangle_q = U_q$ [14,15], where $\hat{\mathcal{H}}$ is the hamiltonian and U_q is a finite quantity (generalized internal energy). We obtain, for q < 1 and $\beta \geq 0$, the generalized equilibrium distribution

$$\hat{\rho} = \begin{cases} [1 - \beta(1-q)\hat{\mathcal{H}}]^{1/(1-q)}/Z_q, & \text{if} \quad 1 - \beta(1-q)\hat{\mathcal{H}} > 0, \\ 0, & \text{otherwise}, \end{cases}$$
(3)

with the generalized partition function given by

$$Z_q = \text{Tr}[1 - \beta(1-q)\hat{\mathcal{H}}]^{1/(1-q)}$$
 , (4)

where the trace concerns only the states for which $\hat{\rho} \neq 0$. In the $q \to 1$ limit, this expression recovers the Boltzmann-Gibbs distribution $\hat{\rho} = \exp(-\beta \hat{\mathcal{H}})/Z_1$. If q > 1, we obtain

$$\hat{\rho} = \begin{cases} [1 - \beta(1 - q)\hat{\mathcal{H}}]^{1/(1 - q)}/Z_q, & \text{if} \quad 1 - \beta(1 - q)E_* > 0, \\ \delta_{*,*}/g_*, & \text{otherwise,} \end{cases}$$
(5)

where $\delta_{\bullet,\bullet}$ is a Kroenecker's delta and

$$(E_{\bullet}, g_{\bullet}) = \begin{cases} (E_l, g_l), & \text{if} \quad \beta \ge 0, \\ (E_h, g_h), & \text{if} \quad \beta \le 0, \end{cases}$$

$$(6)$$

 E_l and g_l being respectively the *lowest* eigenvalue of $\hat{\mathcal{H}}$ and its associated degeneracy, and E_h and g_h being respectively the *highest* eigenvalue of $\hat{\mathcal{H}}$ and its associated degeneracy. In

the $q \to 1$ limit, Eq. (5) recovers, as before, the Boltzmann-Gibbs distribution. Excepting for extremely pathological cases (which are out of the scope of the present work) the negative (positive) temperature region is physically inaccessible unless E_h (E_l) is finite, i.e., if the energy spectrum $\{E_s\}$ has an upper (lower) bound.

It can be shown [15] that, in general,

$$\frac{1}{T} = \frac{\partial S_{\mathbf{q}}}{\partial U_{\mathbf{q}}} \qquad , \tag{7}$$

$$U_q = -\frac{\partial}{\partial \beta} \frac{Z_q^{1-q} - 1}{1-q} \qquad , \tag{8}$$

and

$$F_{q} \equiv U_{q} - TS_{q} = -\frac{1}{\beta} \frac{Z_{q}^{1-q} - 1}{1-q} \qquad (9)$$

In addition to the above properties, the present generalized statistics: (i) leaves form-invariant, for all values of q, the Legendre-transform structure of Thermodynamics [15] as well as the Ehrenfest theorem and the von Neumann equation [17]; (ii) satisfies Jaynes Information Theory duality relations [17] (necessary for the corresponding entropy to be considered as a measure of the (lack of) information); (iii) generalizes the Bogolyubov inequality [19], the Langevin and Fokker-Planck equations [20], the quantum statistics [18], the fluctuation-dissipation theorem [21], the single-site Callen identity [22], the Ising transmissivity [23], among others. The present generalized formalism has been successfully applied (or could be applied) in a variety of problems such as gravitational systems [36-38], anomalous diffusion [39,40], Biology ([41]; see also [29]), Economics [25,42], optimization algorithms [30], statistical inference and Probability Theory [43,44] and learning neural networks [45]. In Section 2 we discuss with some detail some of the above problems; in Section 3 we present the results concerning the infinite-range Ising ferromagnet; we finally conclude in Section 4.

2. Needs for Departure from Boltzmann-Gibbs Statistical Mechanics

The need for departure from Boltzmann-Gibbs statistics becomes nowadays stronger and stronger, and it appears, as already mentioned, in a great variety of physical systems [31-35]. In this Section we discuss three of them, namely, anomalous diffusion (superdiffusion), gravitational-like systems and long-range Ising ferromagnetism (to which this paper is basically dedicated).

2.1. Anomalous Diffusion

In d-dimensional normal diffusion the distance $r \equiv |\vec{r}|$ scales with $t^{1/2}$. However, there are in Nature a variety of systems (alongated micelles [46], heartbeat histograms [47], among many others [48]) which present Lévy-like superdiffusion. In these cases, the distance r scales with $t^{1/\gamma}$ ($0 < \gamma < 2$). To be more precise, if a single jump occurs with probability $\propto 1/r^{d+\mu}$ ($r \to \infty$), then t jumps eventually yield a probability law which, in the $t \to \infty$ limit, provides distances r which scale with $t^{1/\gamma}$ with $\gamma = 2$ if $\mu \ge 2$ and $\gamma = \mu$ if $0 < \mu < 2$. In fact, the generalized central limit theorem [49] implies that the attractor (in probability-law space) is a Lévy distribution; furthermore it is known that γ is the fractal dimension of the Lévy-like diffusion. For the d = 1 case, Alemany and Zanette [39] recently showed that, by optimizing $S_q[p] \equiv \{1 - \int dx \ [p(x)]^q\}/(q-1)$ with $\int dx \ p(x) = 1$ and the simple constraint of fixing $\langle x^2 \rangle_q \equiv \int dx \ x^2 [p(x)]^q$, the correct value of the index q is given by

$$q = \frac{3+\gamma}{1+\gamma} \tag{10}$$

The full discussion of the d = 1 case provides [40]

$$\gamma = \begin{cases} 2, & \text{if } -\infty \le q \le 5/3, \\ (3-q)/(q-1), & \text{if } 5/3 \le q < 3. \end{cases}$$
 (11.a)

Eq. (11.b) is of course consistent with (10). Values of $q \ge 3$ are forbidden since they provide a non-normalizable probability law $(\int dx \ p(x) = \infty)$. The need for $q \ne 1$ statistics comes from the fact that, when q increases from $-\infty$ to 5/3, $\langle x^2 \rangle_1 \equiv \int dx \ x^2 p(x)$ monotonically increases and finally diverges when q approaches 5/3 from below, i.e., for $q \ge 5/3$, fixed $\langle x^2 \rangle_1$ becomes unacceptable as a constraint. In clear constrast, $\langle x^2 \rangle_q$ (which is the natural quantity to be fixed within the generalized statistics) remains finite for all q up to q = 3. For example, $\gamma = 1$ (hence q = 2) corresponds to a Lorentzian distribution $\propto 1/(1+x^2)$: while $\langle x^2 \rangle_1 \propto \int dx \ x^2/(1+x^2)$ diverges, $\langle x^2 \rangle_2 \propto \int dx \ x^2/(1+x^2)^2$ converges! Very recently, Eq. (11) has been extended to d dimensions $(0 \le d \le \infty)$, thus becoming [50]

$$\gamma = \begin{cases} 2, & \text{if} \quad q \le q_c \equiv (4+d)/(2+d), \\ 2/(q-1) - d, & \text{if} \quad q_c \le q < q_{max} \equiv (2+d)/d. \end{cases}$$
 (12.a)

The integral $\int dr \ r^{d-1}p(r)$ diverges if $q \geq q_{max}$. Eq. (12.b) relates q with the fractal dimension γ (i.e., with the long distance behaviour of the probability law $p(r) \propto 1/r^{d+\mu}$ $(r \to \infty)$, with $\gamma = 2$ if $\mu \geq 2$ and $\gamma = \mu$ if $0 < \mu \leq 2$) and the Euclidian dimension d in the cases where Boltzmann-Gibbs (q = 1) fails. Summarizing, we have now a formalism within which all the relevant statistical quantities $(S_q, \langle r^2 \rangle_q, \text{ etc})$ are simultaneously finite (hence, satisfactorily defined!) all the way up to the extreme value $q = q_{max}$ (hence, for $\mu = \gamma$ down to zero!).

2.2. Gravitational-like Systems

Let us address now a d-dimensional N-body gravitational-like problem. More specifically, assume N classical particles interacting attractively through two-body interactions characterized by a potencial V(r) which diverges $(V(r) = +\infty)$ if $r \equiv$ distance between the two particles) is smaller than a cut-off Λ , and which, for $r \geq \Lambda$, is given by

$$V(r) = \begin{cases} A/r^{\alpha}, & \text{if } \alpha \leq 0, \\ A \ln r, & \text{if } \alpha = 0. \end{cases}$$
 (13.a)

Since the interaction is an attractive one, A < 0 if $\alpha \ge 0$ and A > 0 if $\alpha < 0$. The cut-off Λ , which avoids possible r=0 divergences, is physically very natural due to unavoidable quantum effects. A central integral of the Boltzmann-Gibbs discussion of such a system clearly is $\langle V(r) \rangle_1 \propto \int_{\Lambda}^{\infty} dr \ r^{d-1} V(r) \exp[-\beta V(r)]$. This integral diverges if $0 < \alpha < d$, whereas it converges for $\alpha < 0$ and $\alpha > d$ ($\alpha = 0$ and $\alpha = d$ are marginal situations to be discussed on their own). Newtonian d-dimensional gravitation corresponds to $\alpha=d-2$ (solution of the d-dimensional Poisson equation), hence it belongs to the forbidden region if d > 2, in particular for d = 3! (a difficulty which is well known by astrophysicists). The marginal case $(d, \alpha) = (2, 0)$ provides, for the above integral, convergent values for T below a critical value T^* , and divergent values for T above it. Another interesting case is $(d, \alpha) = (3, 3)$, which corresponds essentially to permanent dipole-dipole interactions. Its marginality is reflected into the well-known (nevertheless bizarre within an extensive thermodynamic formalism) fact that calculations of total polarization (and related quantities) depend on the external shape of the sample! The whole situation is depicted in Fig. 1, and can be summarized by saying that Boltzmann-Gibbs statistics (q = 1) is the correct frame if $\alpha < 0$ or if $\alpha > d$ (with some precautions we can even extend its validity to $\alpha \leq 0$ or $\alpha \geq d$), but if $\alpha \in (0,d)$ we no doubt need nonextensive statistics $(q \neq 1 \text{ within }$ the present proposal). By analogy with what was presented in Section 2.1, one naturally expects q to depend on (d, α) if $0 < \alpha < d$, but unfortunately the precise relation is not yet available.

Let us now address the question of whether the correct value of the index q for the present system is above of below 1. Plastino and Plastino [36] as well as Aly [37] discussed d=3 gravitation (i.e., $\alpha=1$) and established (Plastino and Plastino for the polytropic model and Aly through quite general arguments) that q must be above 9/7 in order to have values for the mass, the energy and the entropy which are simultaneously finite. However, a correction is needed. Indeed, both papers [36] and [37] used an early form (presented in [14]) of the generalized statistics where, to each observable \hat{O} , one associates the mean value $\langle \hat{O} \rangle_1 \equiv \text{Tr} \hat{\rho} \ \hat{O}$ with $\hat{\rho} \propto [1 - \beta(q-1)\hat{\mathcal{H}}]^{1/(q-1)}$. However, the relevant form is now known to be the q-expectation value $\langle \hat{O} \rangle_q \equiv \text{Tr} \hat{\rho}^q \hat{O}$ with $\hat{\rho} \propto [1 - \beta(1-q)\hat{\mathcal{H}}]^{1/(1-q)}$ (as tackled in [14] and presented in [15]). Consequently, the correct discussion is to be

done on

 $\langle \hat{O} \rangle_q = Z_q^{-q} \, \operatorname{Tr} \{ [1 - \beta (1-q) \hat{\mathcal{H}}]^{q/(1-q)} \, \hat{O} \} = Z_q^{-q} \, \operatorname{Tr} \{ [1 - \beta q (1/q \, -1) \hat{\mathcal{H}}]^{1/(1/q \, -1)} \, \hat{O} \} \, \, \text{with} \, \,$ $Z_{q} \equiv \text{Tr}[1-\beta(1-q)\hat{\mathcal{H}}]^{1/(1-q)} \text{ , and not on } \langle \hat{O} \rangle_{1} = Z_{q} \text{ Tr}\{[1-\beta(q-1)\hat{\mathcal{H}}]^{1/(q-1)}\hat{O}\} \text{ with } Z_{q} \equiv 2\pi i \{[1-\beta(q-1)\hat{\mathcal{H}}]^{1/(q-1)}\hat{O}\}$ $\text{Tr}[1-\beta(q-1)\hat{\mathcal{H}}]^{1/(q-1)}$. There is no simple and general connection between the correct (β,q) dependence of $\langle \hat{O} \rangle_q$ and that of the above $\langle \hat{O} \rangle_1$. It is however clear that if unsatisfactory divergent integrals are found, within the early approach, by Plastino and Plastino and by Aly for q < 9/7, the same type of difficulties are expected to appear, within the corrected approach, for q > 7/9. Summarizing, the physically correct discussion of the d=3 gravitation is to be done for q<7/9 (hence q<1). This result has been recently re-inforced by a discussion [38] of the d=3 gravitation Vlasov equation. Indeed, the exact time-dependent solutions of the homogeneous density slabs and of the Freeman-like rigid disk models of stellar matter are available since 1973 [51] and 1990 [52] respectively. These rather complex time-dependent solutions have been exactly recovered by Plastino and Plastino [38], for both models, within the framework of the generalized Statistical Mechanics by using q = -1 (hence q < 1). Finally, the demand for entropy superadditivity which appears to be necessary in the discussion of black holes (see Landsberg 1984 [31]) occurs here (see Eq. (2)) only if q < 1.

2.3. Long-Range Ising Ferromagnetism

The Hamiltonian we now focus is

$$\mathcal{H} = -2\sum_{(i,j)} J_{ij} S_i S_j \qquad (S_i = \pm 1, \ \forall i) \qquad , \tag{14}$$

with

$$J_{ij} = J/\tau_{ij}^{d+\delta} \qquad (J > 0 ; d+\delta \ge 0) \qquad , \tag{15}$$

where r_{ij} is the distance (in crystal units) between sites i and j, and where the sum $\sum_{(i,j)}$ runs over all N(N-1)/2 distinct pairs of sites on a d-dimensional simple hypercubic

lattice $(d = 1 \text{ yields } r_{ij} = 1, 2, 3, \cdots; d = 2 \text{ yields } r_{ij} = 1, \sqrt{2}, 2, \sqrt{5}, \cdots; d = 3 \text{ yields } r_{ij} = 1, \sqrt{2}, \sqrt{3}, 2, \cdots)$. The limit $\delta \to \infty$ corresponds to the d-dimensional first-neighbor model. The $d + \delta = 0$ particular case corresponds to the infinite-range (hence, dimensionless) ferromagnet, i.e., basically the Mean-Field Approach (MFA); the MFA can also be attained in the the $d \to \infty$ limit, $\forall \delta$. The critical temperature $T_c(d, \delta)$ of this model satisfies: (i) $T_c(d, \infty)$ monotonically varies from zero to infinity when d increases from 1 to infinity (no phase transition exists for $0 \le d < 1$; $k_B T_c(1, \infty)/2J = 0$; $k_B T_c(2, \infty)/2J = 2.269...[53]$; $k_B T_c(d, \infty)/2J \sim 2d$ if $d \to \infty$); (ii) $k_B T_c(d, -d)/2J = \infty$, $\forall d$ (if we follow say the specific heat peak while the number N of spins diverges, then $k_B T_c(d, -d)/2J \sim N$ [54]); (iii) $k_B T_c(\infty, \delta)/2J = \infty$, $\forall \delta$ (once more $k_B T_c(\infty, \delta)/2J \sim N$ in the $N \to \infty$ limit). The fact that, in all these results, 2J appears instead of the standard coupling constant J comes from the notation adopted in Eq. (14); this notation follows that of Ref. [54], where the infinite-range model is discussed.

Let us discuss the Boltzmann-Gibbs internal energy $U_1 \equiv \langle \mathcal{H} \rangle_1 = -2J \sum_{(i,j)} (1/r_{ij}^{d+\delta}) \times \langle S_i S_j \rangle_1$. At T=0 the fundamental state (either $S_i=1$, $\forall i$, or $S_i=-1$, $\forall i$) is the only one to be occupied, hence

$$-\frac{U_1}{J} = 2\sum_{(i,j)} \frac{1}{r_{ij}^{d+\delta}} = N\sum_j \frac{1}{r_{ij}^{d+\delta}} \qquad (16)$$

At long distances this sum can essentially be replaced by

$$\int_{1}^{\infty} dr \ r^{d-1}(1/r^{d+\delta}) \qquad , \tag{17}$$

which diverges for $\delta \leq 0$. In other words, one expects $k_BT_c(d,\delta)/J$ to diverge when $\delta \to +0$ and remain infinite for $\delta \leq 0$. Let us quote the words of Hiley and Joyce [55] who focused this problem in 1965: "With $\delta < 0$ this sum (essentially Eq. (16)) is divergent and, in consequence, the properties of a model using this type of potential will be non-thermodynamic. We will, therefore, not discuss these models further". They also point that, for $\delta = 0$, conditionally convergent series appear and the results depend on "the shape of the specimen", as for the permanent dipole-dipole interaction we discussed

in Section 2.2 . Consequently, Hiley and Joyce concentrate on the $\delta > 0$ case, very especially in the $\delta \to +0$ limit, where the discussion becomes tractable. Once more, it becomes obvious the need, for $\delta < 0$, of nonextensive thermodynamics $(q \neq 1)$ within the present proposal). The natural proposal is a (d, δ) -dependent index q (possibly $q(d, \delta) < 1$ if $\delta < 0$ in analogy with the gravitational case). The whole situation is depicted in Fig. 2, where we have incorporated: (i) the well-known fact that, for d > 4, the phase transition exponents are the so-called classical or Landau ones; (ii) the fact that $\delta \geq 2$ implies short-range interactions (since the Fourier transform of $1/r^{d+\delta}$ is proportional to $\exp\{-\text{constant}(\text{wavevector})^2\}$), hence the universality classes are those of the first-neighbor models; (iii) the crossover from the short-range to the long-range universality which occurs [56] at $\delta = d/2$.

In order to start exploring, within $q \neq 1$ thermostatistics, the unusual region $\delta < 0$, we concentrate in what follows on the *infinite-range model* (i.e., $d + \delta = 0$).

3. Infinite-Range Ising Ferromagnet

From now on we address the Hamiltonian

$$\mathcal{H} = -2\sum_{(i,j)} J_{ij} S_i S_j + JB \qquad (J > 0) \qquad , \tag{18}$$

where we have added a constant JB to Hamiltonian (14). Eq. (18) can be rewritten as follows:

$$\mathcal{H} = -J \sum_{i=1}^{N} \sum_{j=1}^{N} S_i S_j + JN + JB$$

$$= -J \left(\sum_{i=1}^{N} S_i \right)^2 + JN + JB \qquad . \tag{19}$$

For simplicity, from now on we assume N even. If we introduce now $\sum_{i=1}^{N} S_i \equiv N_{\uparrow} - N_{\downarrow}$

and $N = N_1 + N_1$ we have the following dimensionless spectrum for \mathcal{H} (in units of J):

$$E_{N_1} = -(2N_1 - N)^2 + N + B$$
 $(N_1 = 0, 1, 2, \dots, N)$, (20)

associated with a "degeneracy" $N!/[N_1!(N-N_1)!]$ (strictly speaking, since we have no external magnetic field, we could restrict N_1 to vary from 0 to N/2, all levels having a degeneracy $2N!/[N_1!(N-N_1)!]$ excepting that corresponding to $N_1 = N/2$ which has a degeneracy $N!/[(N/2)!]^2$). The dimensionless energy of the fundamental level (all spins parallel) equals $-N^2 + N + B \equiv E_{min}$, that of the most excited level (half spins up and half down) equals $N + B \equiv E_{max}$, hence the width of the spectrum equals N^2 . This fact hopefully determines the correct scaling for the temperature, which is, as we shall verify later on, kT/N^2J if $q \neq 1$ and k_BT/NJ if q = 1. Three typical choices exist for B, namely: nonnegative spectrum $(E_{min} = 0$, hence B = N(N-1)), nonpositive spectrum $(E_{max} = 0$, hence B = -N), and mixed spectrum $(E_{min} = -E_{max})$, hence B = N(N-2)/2. In the present paper, we discuss, for positive temperatures, the specific heat associated with all three cases for $q \geq 1$, and exhibit that the thermodynamic limit $(N \to \infty)$ is well defined; in other words, it yields (in properly scaled specific heat and temperature) functions which are finite almost everywhere.

q=1:

The specific heat independs from B and is given by

$$\frac{C_1}{k_B} = \left(\frac{J}{k_B T}\right)^2 \left\{ \sum_{N_1=0}^{N} \frac{N!}{N_1!(N-N_1)!} p_{N_1} E_{N_1}^2 - \left[\sum_{N_1=0}^{N} \frac{N!}{N_1!(N-N_1)!} p_{N_1} E_{N_1} \right]^2 \right\} ,$$
(21)

where

$$p_{N_{\dagger}} = \frac{1}{Z_{1}} \exp\left(-\frac{J}{k_{B}T} E_{N_{\dagger}}\right) \qquad , \tag{22}$$

with

$$Z_{1} = \sum_{N_{1}=0}^{N} \frac{N!}{N_{1}!(N-N_{1})!} \exp\left(-\frac{J}{k_{B}T} E_{N_{1}}\right) \qquad (23)$$

The numerically exact results for increasingly large systems are presented in Fig. 3. A phase transition emerges, in the limit $N \to \infty$, with a critical temperature given by $k_B T_c/NJ = 2$.

q < 1:

The specific heat depends on B and is given by [21,25,26]

$$\frac{C_{q}}{k} = q \left(\frac{J}{kT}\right)^{2} \left\{ \sum_{N_{1}=0}^{N} \frac{N!}{N_{1}!(N-N_{1})!} p_{N_{1}}^{q} \frac{E_{N_{1}}^{2}}{1-(J/kT)(1-q)E_{N_{1}}} - \left[\sum_{N_{1}=0}^{N} \frac{N!}{N_{1}!(N-N_{1})!} p_{N_{1}}^{q} E_{N_{1}} \right] \left[\sum_{N_{1}=0}^{N} \frac{N!}{N_{1}!(N-N_{1})!} p_{N_{1}} \frac{E_{N_{1}}}{1-(J/kT)(1-q)E_{N_{1}}} \right] \right\} , \tag{24}$$

where

$$p_{N_{\uparrow}} = \begin{cases} [1 - (J/kT)(1 - q)E_{N_{\uparrow}}]^{1/(1 - q)}/Z_q, & \text{if } 1 > (J/kT)(1 - q)E_{N_{\uparrow}}, \\ 0, & \text{otherwise}, \end{cases}$$
 (25)

with

$$Z_{q} = \sum_{N_{1}=0}^{N} \frac{N!}{N_{1}!(N-N_{1})!} \left[1 - \frac{J}{kT} (1-q) E_{N_{1}} \right]^{1/(1-q)}$$
 (26)

By \sum' we mean that the sum is interrupted whenever the restriction $1 > (J/kT)(1-q)E_{N_1}$ is violated.

The numerically exact results for increasingly large systems are presented in Figs. 4-6. Once again a phase transition emerges, in the $N \to \infty$ limit, if $E_{max} \ge 0$ (i.e., if $N + B \ge 0$), and its critical temperature is given by

$$\frac{kT_c}{N^2J} = (1-q) \frac{E_{max}}{E_{max} - E_{min}} = (1-q) \frac{N+B}{N^2} \qquad . \tag{27}$$

If $E_{max} < 0$ (i.e., if N+B < 0), no phase transition exists (at least, no divergence exists in the $N \to \infty$ limit of the rescaled specific heat). Also, if $-N^2+N+B>0$, we have a forbidden region (physically inaccessible) for $kT/J \in [0,(1-q)(-N^2+N+B)]$, a frozen region (zero specific heat) for $kT/J \in ((1-q)(-N^2+N+B),(1-q)[-(N-2)^2+N+B]]$, and an active region (nonzero specific heat) for $kT/J > (1-q)[-(N-2)^2+N+B]$. If $-N^2+N+B<0<-(N-2)^2+N+B$, we have a frozen region for $kT/J \le (1-q)[-(N-2)^2+N+B]$, and an active region otherwise. Finally, if $-(N-2)^2+N+B<0$, the system is active for all positive temperatures.

A simple choice for B in the $N\to\infty$ limit is $B+N=\eta N^2$, η being a pure number $(\eta=0,1/2)$ and 1 respectively correspond to nonpositive, mixed and nonnegative spectra). In this case: (i) there is evidence for a phase transition only for $\eta\geq 0$, and the critical point satisfies $kT_c/N^2J=(1-q)\eta$; (ii) there is a finite forbidden region only if $\eta>1$, and corresponds to $kT/N^2J\leq (1-q)(\eta-1)$ (above this point, the system is thermally active).

q>1:

The specific heat depends on B and is given by Eq. (24) where

$$p_{N_{\uparrow}} = \begin{cases} \left\{ [1 + (J/kT)(q-1)E_{N_{\uparrow}}]^{1/(q-1)} Z_{q} \right\}^{-1}, & \text{if } 1 + (J/kT)(q-1)E_{min} > 0, \\ (\delta_{N_{\uparrow},0} + \delta_{N_{\uparrow},N})/2, & \text{otherwise}, \end{cases}$$
(28)

(δ refers to Kroenecker's delta) with

$$Z_{q} = \sum_{N_{1}=0}^{N} \frac{N!}{N_{1}!(N-N_{1})!} \left\{ \left[1 + \frac{J}{kT}(q-1)E_{N_{1}} \right]^{1/(q-1)} \right\}^{-1}$$
 (29)

As before, the sum is restricted to N_{\uparrow} such that $1 + (J/kT)(q-1)E_{N_{\uparrow}} > 0$. If $E_{min} \ge 0$, then, for all positive temperatures, the system is thermally active; if $E_{min} < 0$, the system is active only for kT/J above $(q-1)|E_{min}|$, being frozen below.

The numerically exact results for increasingly large systems are presented in Figs. 7-9. There is no evidence for a phase transition in none of these cases.

If we have $(B+N)/N^2=\eta\in\Re$ in the $N\to\infty$ limit, the temperature above which the system is frozen is given by $kT_F/N^2J=(q-1)(1-\eta)$ if $\eta<1$, and the temperature T_{max} at which the rescaled specific heat attains a soft maximum is given by $kT_{max}/N^2J=(q-1)\eta/2$. Consequently, $N^2C_q/2^{(1-q)N}k$ achieves its physically meaningful maximum at T_F (with $dC_q/dT|_{T_F}<0$) if $\eta<2/3$, at $T_F=T_{max}$ (with $dC_q/dT|_{T_{max}}=0$) if $\eta>2/3$, and at T_{max} (with $dC_q/dT|_{T_{max}}=0$) if $\eta>2/3$.

4. Conclusion

We have discussed the validity limits of extensive thermostatistics (i.e., Boltzmann-Gibbs Statistical Mechanics and standard Thermodynamics) in three important systems, namely Lévy-like anomalous diffusion, gravitational-like models and long-range Ising ferromagnets. The unified picture which emerges is that, whenever Boltzmann-Gibbs formalism (q = 1) fails, the problem hopefully becomes tractable within nonextensive thermostatistics $(q \neq 1)$. The index q is shown, for the Lévy problem, to depend only on the

space dimensionality d and the power characterizing the long-range interactions. This is expected to be also true for the gravitational and magnetic cases herein focused.

We have then addressed the thermal dependence (for positive temperatures) of the specific heat associated with the infinite-range spin 1/2 Ising ferromagnet, i.e., N spins interacting (two by two) all with all. Our numerically exact results (summarized in the Table) strongly suggest a variety of phenomena in the limit $N \to \infty$. Let us mention here the most remarkable two:

- (i) in complete analogy with the well known C_1/Nk_B vs. k_BT/N curves within Boltzmann-Gibbs statistics (q=1), the curves $N^2C_q/2^{(1-q)N}k$ vs. kT/N^2J within $q \neq 1$ statistics tend to a numerically well defined thermodynamic limit; this is the first time that the existence of such a limit is exhibited for an interacting model (this fact has already been verified for a noninteracting model [29]);
- (ii) analogously with the Landau-like phase transition which is known to exist for q=1, a nontrivial divergence, at a finite rescaled temperature, in the rescaled specific heat is observed for 0 < q < 1 (not for q > 1) whenever the energy spectrum includes a positive portion. Although no evidence for phase transitions has been obtained for q > 1, these should not be excluded without further studies. Indeed, the specific heat critical exponent α is herein shown to be positive for q < 1, and it is known to be zero for q = 1 (MFA). Consequently, it could well be that it is negative for q > 1, thus producing a soft thermal dependence of the specific heat (as herein observed!).

Acknowledgments

One of us (C.T.) is greatly indebted with A.M.C. de Souza and with N. Boccara for extremely valuable discussions on the Lévy problem and the figure 2 respectively; he also acknowledges with pleasure warm hospitality received at the Universidade Federal do Rio Grande do Norte. We thank CNPq and CAPES (Brazilian agencies) for partial financial support.

Captions for Figures and Table

- Fig. 1: d-dimensional gravitational-like systems (with attractive potential $\propto r^{-\alpha}$ at long distances; see Eq. (13)). Boltzmann-Gibbs statistics (q=1) is fully satisfactory for $\alpha > d$ and $\alpha < 0$, marginally satisfactory for $\alpha = d$ and $\alpha = 0$, and unsatisfactory for $0 < \alpha < d$ (where it should hopefully be replaced by nonextensive statistics with q possibly below unity). Standard d-dimensional gravitation corresponds to $\alpha = d-2$. We have used the expression "quasi-ideal gas" rather than "ideal gas" for the d=0 axis because of the presence of a non-vanishing short-distance cut-off Λ ("ideal gas" would strictly correspond to $\Lambda=0$). $d=\alpha=3$ corresponds to the permanent dipole-dipole interaction, excepting for the angular effects.
- Fig. 2: d-dimensional spin 1/2 long-range Ising ferromagnet $(J_{ij} = Jr_{ij}^{-(d+\delta)}; d+\delta \geq 0;$ see Eqs. (14) and (15)). Boltzmann-Gibbs statistics (q=1) is fully satisfactory for $\delta > 0$, marginally satisfactory for $\delta = 0$ and unsatisfactory for $\delta < 0$ (where it should hopefully be replaced by nonextensive statistics with q possibly below unity). The $T_c = 0$ dashed line (joining the point $(d, d+\delta) = (1,3)$ with the origin) is only indicative since the exact answer is, to the best of our knowledge, still unknown. The Mean Field Approach (MFA) corresponds to both $d+\delta \to 0$ ($\forall d$) and $d \to \infty$ ($\forall d+\delta > 0$); the first-neighbor models correspond to $d+\delta \to \infty$ ($\forall d$); the ideal paramagnet (independent localized spins) corresponds to $d \to 0$ ($\forall d+\delta > 0$; see [29]). In the entire region $\delta \leq 0$, the Boltzmann-Gibbs critical temperature diverges. The short- to long-range crossover line corresponds to $d+\delta = d+2$, and the long-range to classical one corresponds to $d+\delta = 3d/2$.
- Fig. 3: Infinite-range model (MFA of Fig. 2) within Boltzmann-Gibbs statistics (q = 1). Both the specific heat C_1 and the temperature T must be rescaled as shown in order to have, in the $N \to \infty$ limit, finite values almost everywhere. The exact $N \to \infty$ rescaled specific heat (dashed line) strictly vanishes if $k_BT/NJ > 2$, and tends to 3/2 if $k_BT/NJ \to (2-0)$ (see [54]).

- Fig. 4: Infinite-range model within q < 1 statistics for nonnegative spectrum (B = N(N-1)) for typical values of q. Both the specific heat C_q and the temperature T must be rescaled as shown in order to have, in the $N \to \infty$ limit, finite values almost everywhere. The insets show the N = 800 full curves.
- Fig. 5: Infinite-range model within q < 1 statistics for mixed spectrum (B = N(N 2)/2) for typical values of q. The insets show the N = 800 full curves.
- Fig. 6: Infinite-range model within q < 1 statistics for nonpositive spectrum (B = -N) for typical values of q. N takes the values 20, 40, 100, 200, 400, 600 and 800. The insets show the N = 800 full curves.
- Fig. 7: Infinite-range model within q > 1 statistics for nonnegative spectrum (B = N(N-1)) for typical values of q. N takes the values 40, 100, 200, 400, 600 and 800.
- Fig. 8: Infinite-range model within q > 1 statistics for mixed spectrum (B = N(N 2)/2) for q = 2. N takes the values 10, 20, 40, 100, 200, 400, 600 and 800.
- Fig. 9: Infinite-range model within q > 1 statistics for nonpositive spectrum (B = -N) for q = 2. N takes the values 10, 20, 40, 100, 200, 400, 600 and 800.
- Table: Summarized results of the present paper. C_1/Nk_B vs. k_BT/NJ independs from B. We use "No evidence for phase transition" in the sense that no divergence appears, in the $N\to\infty$ limit, in the rescaled specific heat as a function of the rescaled temperature. If $(B+N)/N^2=\eta\in\Re$, then q<1 yields $\lim_{N\to\infty}(kT_c/N^2J)=\eta(1-q)$ if $\eta\geq 0$, and q>1 yields $\lim_{N\to\infty}(kT_F/N^2J)=(1-\eta)(q-1)$ if $\eta\leq 1$ and $\lim_{N\to\infty}(kT_{max}/N^2J)=\eta(q-1)/2$ if $\eta\geq 2/3$; these expressions have been numerically checked for arbitrary values of η .

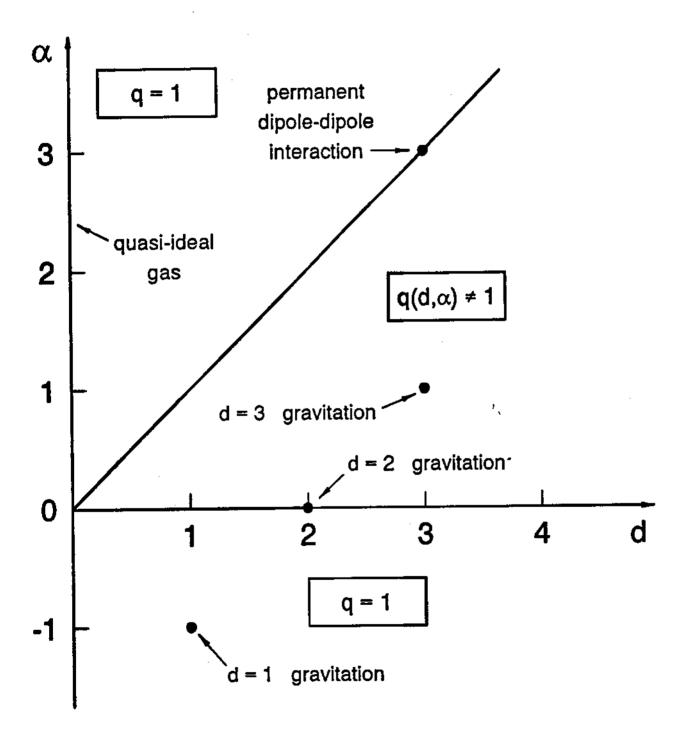


Fig. 1

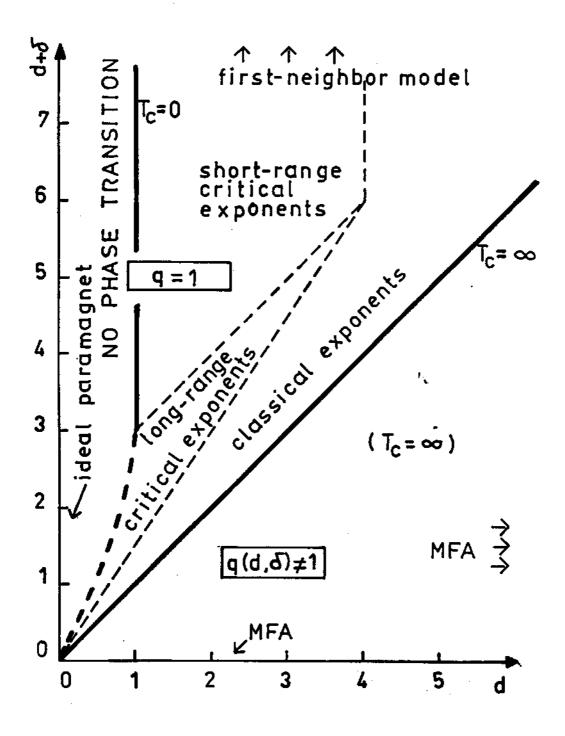
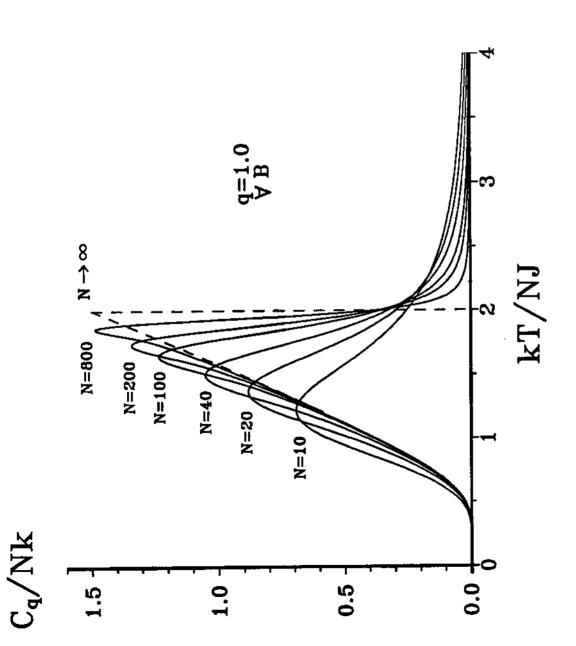


FIG.2





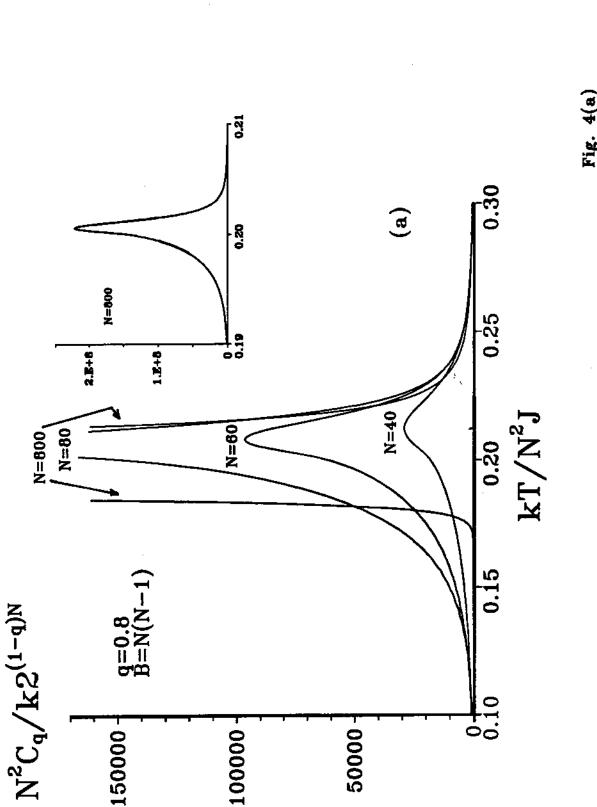


Fig. 4(a) Nobre and Tsallis

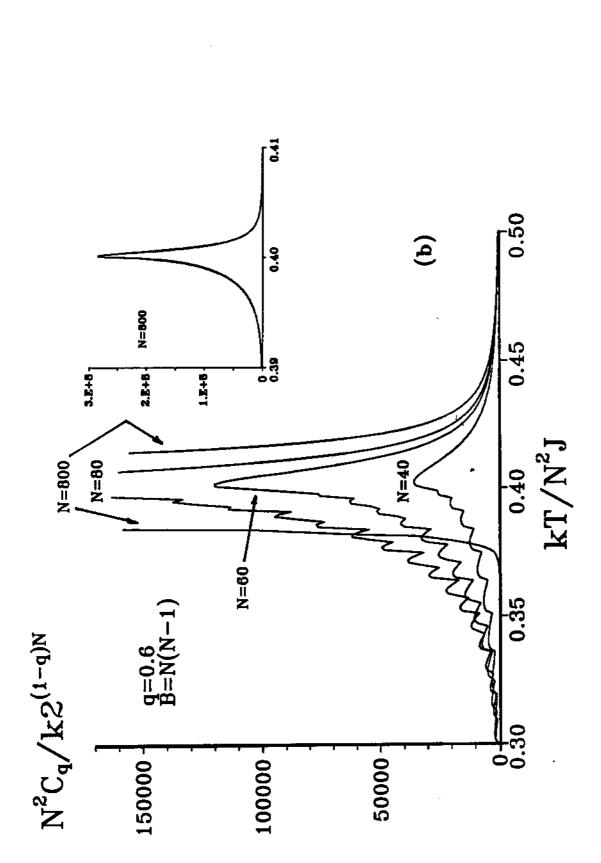
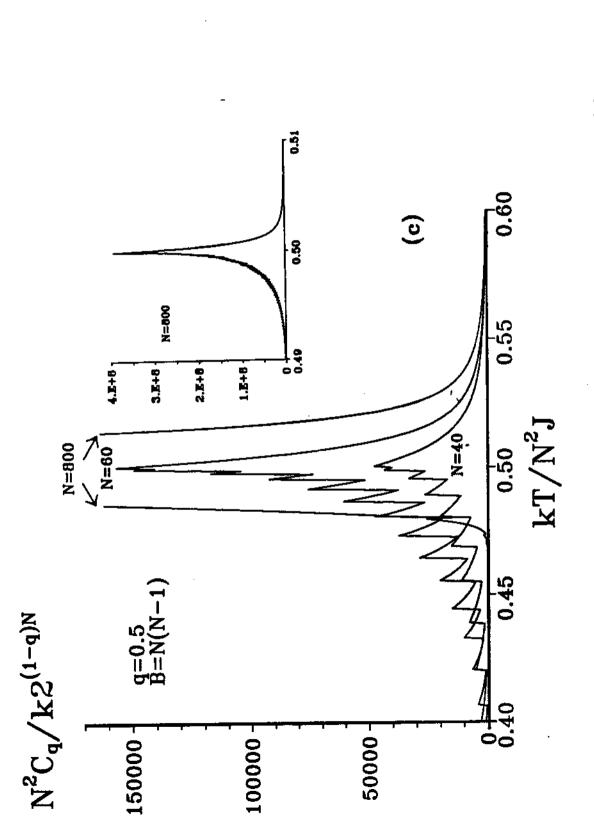
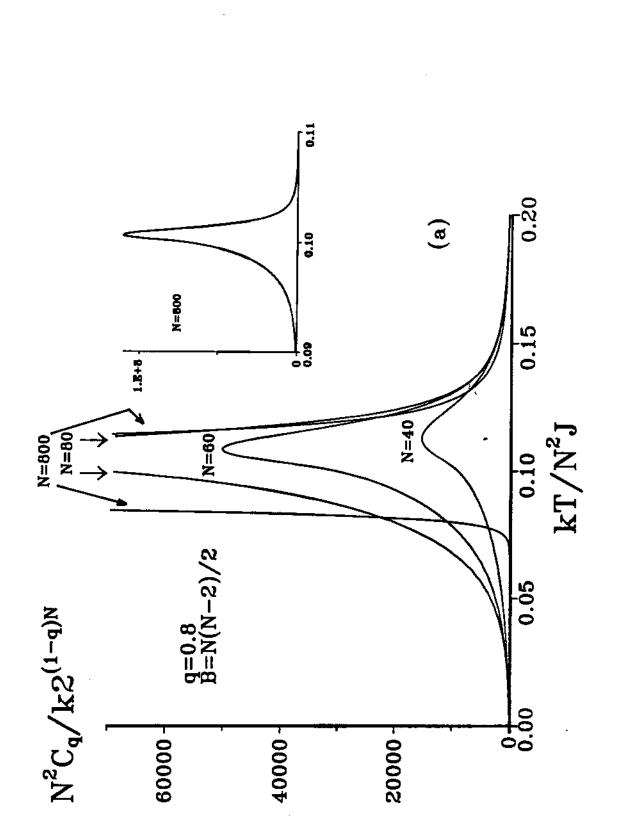


Fig. 4(b) Nobre and Tsallis









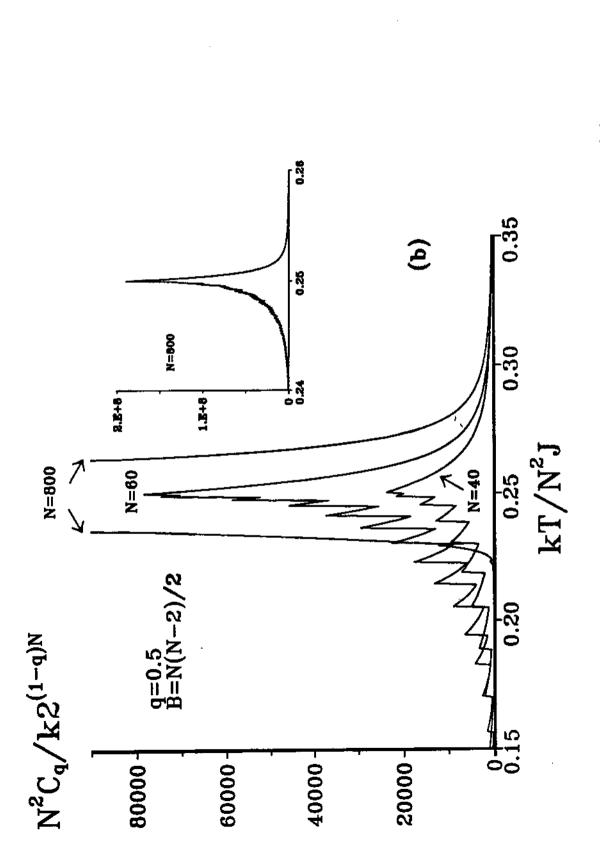
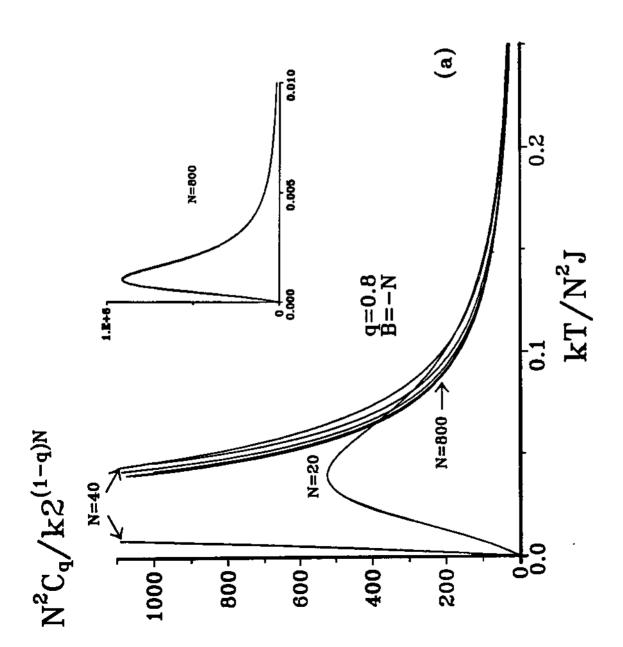


Fig. 5(b) Nobre and Tsallis







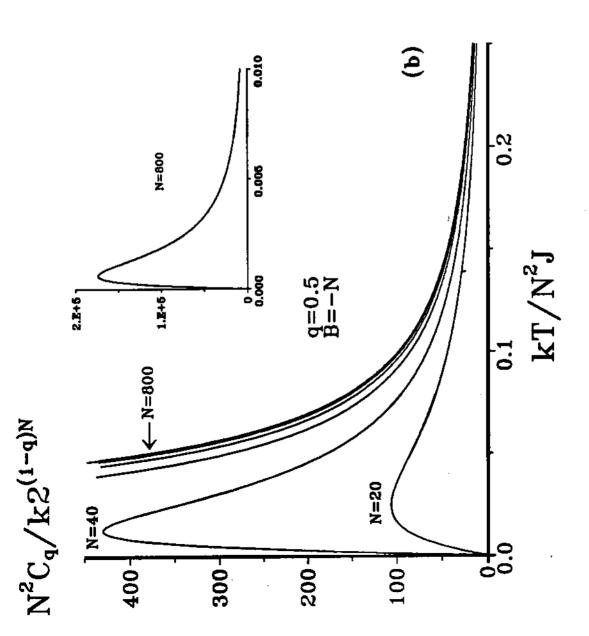
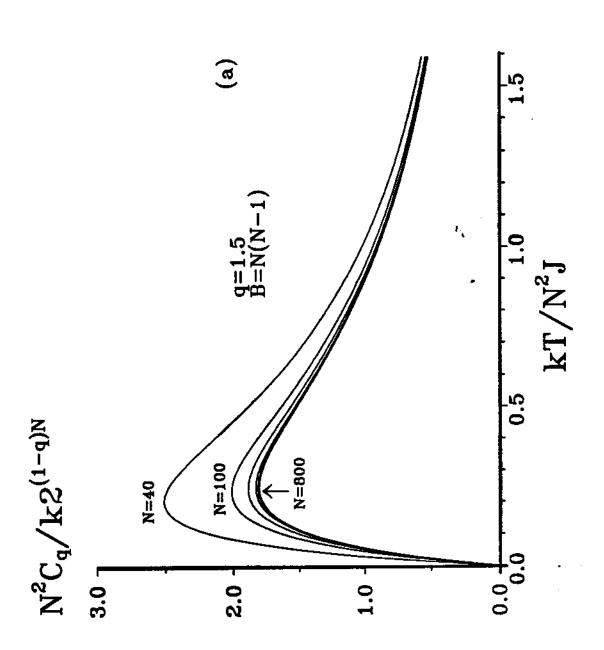
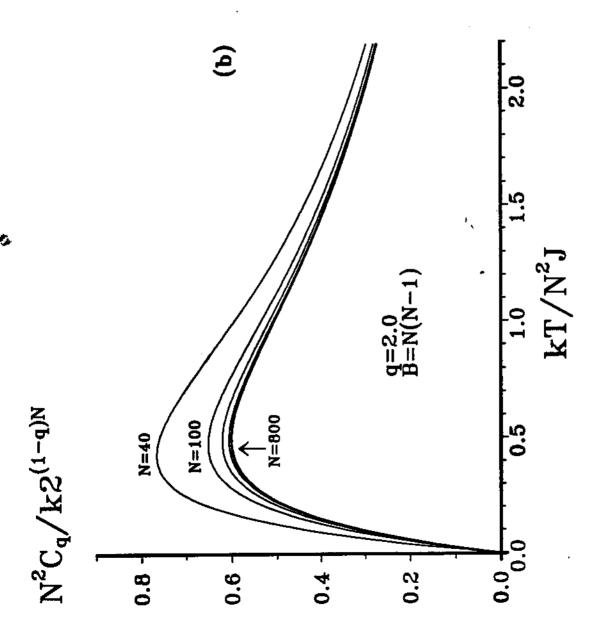


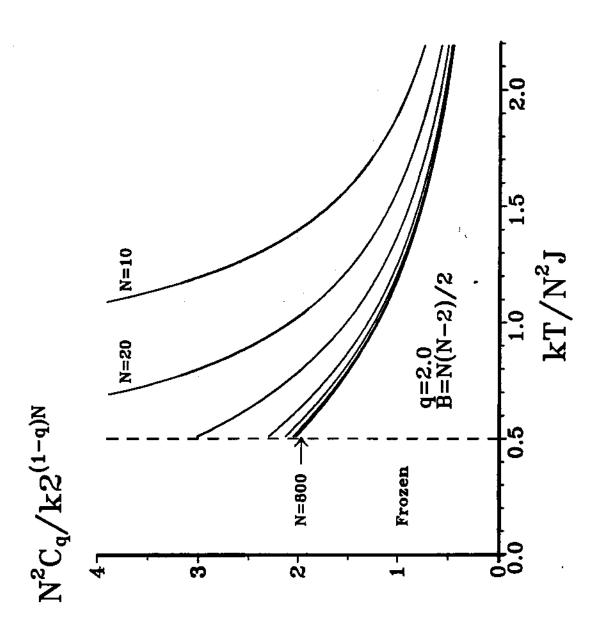
Fig. 7(a) Nobre and Tsallis



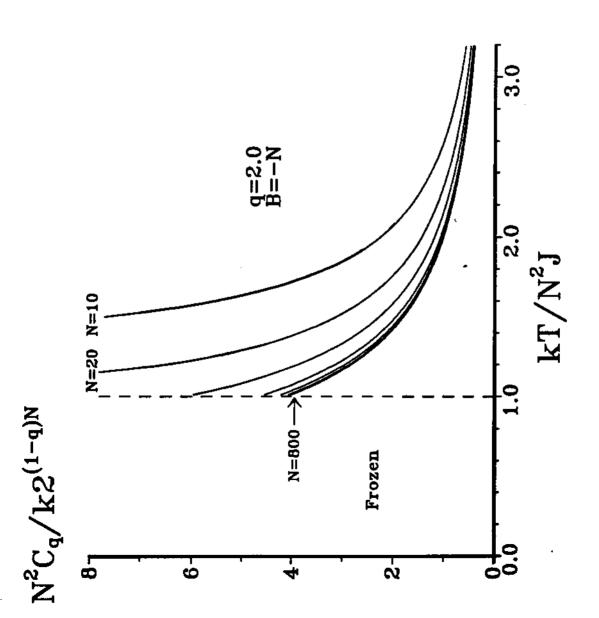












Table

	0 < q < 1	q=1	q > 1
Nonnegative	$N^2C_q/k2^{(1-q)N}$	C_1/k_BN	$N^2C_q/k2^{(1-q)N}$
Spectrum	vs. kT/N^2J	vs. k_BT/NJ	vs. kT/N^2J
(B=N(N-1),		·	
i.e., $\eta = 1$)			No evidence for
	Phase transition	Phase transition	phase transition
,	$\lim_{N\to\infty} (kT_c/N^2J)$	$\lim_{N\to\infty}(k_BT_c/NJ)=2$	$\lim_{N\to\infty}(kT_{max}/N^2J)$
	=1-q		= (q-1)/2
	No frozen region	No frozen region	No frozen region
Mixed	$N^2C_q/k2^{(1-q)N}$	C_1/k_BN	$N^2C_q/k2^{(1-q)N}$
Spectrum	vs. kT/N^2J	vs. k_BT/NJ	vs. kT/N^2J
(B=N(N-2)/2,			
i.e., $\eta = 1/2$)	Phase transition	Phase transition ,	No evidence for
	$\lim_{N\to\infty} (kT_c/N^2J)$	$\lim_{N\to\infty}(k_BT_c/NJ)=2$	phase transition
	= (1-q)/2		•
	No frozen region	No frozen region	Frozen if
			$(kT/N^2J) < (q-1)/2$
Nonpositive	$N^2C_q/k2^{(1-q)N}$	C_1/k_BN	$N^2C_q/k2^{(1-q)N}$
Spectrum	vs. kT/N^2J	vs. k_BT/NJ	vs. kT/N^2J
(B=-N,			
i.e., $\eta = 0$)	Phase transition	Phase transition	No evidence for
	$\lim_{N\to\infty}(kT_c/N^2J)=0$	$\lim_{N\to\infty}(k_BT_c/NJ)=2$	phase transition
	No frozen region	No frozen region	Frozen if
			$(kT/N^2J) < q-1$

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