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Tsallis-Statistical Approach to the Specific Heat of Liquid ^{4}He–Comparison With Other Results.*

by

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ABSTRACT

A theoretical approach [M.R-Monteiro *et al.*, Phys. Rev. Lett. **76**, 1098 (1996)] within a quantum-group formalism ($q_{QG} \neq 1$) has recently been proposed and successfully compared to Greywall's high precision measurements of the liquid ^{4}He specific heat. We calculate here the specific heat for ^{4}He using Tsallis non-extensive thermostatistics ($q_T \neq 1$). A comparative analysis reveals that more sophisticated theories, possibly including many-body interactions, would be necessary for discriminating between alternative formalisms.

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The specific heat of liquid ^{4}He has been measured with high precision [1, 2] for the temperature range $0.14 \leq 0.86$ and values for phonon parameters were determined from experimental data. They also obtained roton parameter from neutron measurements. The low temperature ^{4}He specific heat is usually given by

$$C = C^{Phonon} + C^{Roton} \tag{1}$$

where C^{Phonon} is the polynomial expansion

$$C^{Phonon} = AT^3 + BT^5 + DT^7 \tag{2}$$

that was fitted to the measured values of the specific heat C_E (where E stands for experimental) thus determining the parameters A, B and D; T is the temperature; C^{Roton} is a function of (Δ/k_BT), where Δ is the energy gap [3] and k_B the Boltzmann constant.

In FIG.1., the relative contributions of the phonons (dashed line) and rotons (solid line) are depicted. We can see that for $T < 0.5K$, the roton contribution is smaller than 1%. When T increases from $0.5K$ to $0.8K$ the roton contribution grows very fast and, at $T \approx 0.8K$ both contributions are similar; for temperatures immediately above this value, the roton contribution is the most important one.

Recently, a quantum group (q_{QG}-Bosonic) model [4] for the specific heat (C_{QG}) of ^{4}He has been proposed. The model does not consider inter-particle interactions, i.e., the phonons and rotons are assumed as independent quasi-particles. The phonons are treated as bosonic q_{QG}-oscillators, the rotons as usual. Bosonic q_{QG}-oscillators [5] are a generalization of the Heisenberg algebra by introducing a deformation parameter q_{QG}, where $q_{QG} = 1$ corresponds to the standard quantum mechanic description. The q-deformation of the Heisenberg algebra in the phonon calculation is used to give an algebraic interpretation for the polynomial expansion (2).

On the other hand, Tsallis [6] has presented a generalized thermostatistics, pointing to systems with non-extensive properties. The formalism is dependent on a parameter here denoted by q_T. A possible connection between Tsallis thermostatistics (characterized by $q_T \neq 1$) and quantum group (characterized by $q_{QG} \neq 1$) has been recently proposed [7]. Through the discussion of the mean values of observables, a possible temperature dependent relation between q_T and q_{QG} was derived; it was illustrated with bosonic oscillators.

The aim of the present work is essentially two-fold: (i) to establish the generalized thermostatistic formulation, and (ii) to compare the available different theoretical approaches, for low-temperature phonon excitations in ^{4}He.

Let us denote by $C(q_T, q_{QG}, T)$ the generic specific heat of ^{4}He, where T is the temperature. The possibilities for C are:

$$C(q_T, q_{QG}, T) \rightarrow \begin{cases} C(1,1,T) \equiv C_{BG} & \text{Boltzmann-Gibbs statistics,} \\ C(1,q_{QG},T) \equiv C_{QG} & \text{quantum group,} \\ C(q_T,1,T) \equiv C_T & \text{Tsallis statistics.} \end{cases} \tag{3}$$

In this communication, we first calculate the specific heat C_{BG} using Boltzmann-Gibbs statistics and considering an anomalous phonon dispersion. Then, we obtain a generalized specific heat C_T in the approximation of small departures from the standard model. Finally, we compare our result to those of the q_{QG}-Bosonic model C_{QG} and to experimental data C_E [2].

In a global sense, the Boltzmann-Gibbs thermostatistics and its connection with thermodynamics are powerful tools in theoretical physics to study situations where the following conditions appear (i) the effective microscopic interaction is short-range or inexistent, (ii) the microscopic memory is short-ranged or inexistent and (iii) the system evolves in an euclidean-like (non-fractal) space-time. That is, whenever the extensive (additive) description of thermodynamics holds. Then, we calculate the specific heat without any extra approximation in the Boltzmann-Gibbs framework, considering only the contributions due to phonons and rotons.

We take the Hamiltonian $\mathcal{H}$ for a non-interacting phonon gas, into a box of side ℓ in D dimensions, as given by

$$\mathcal{H} = \hbar \sum_{i=1}^{N} \omega_i (\mathcal{N} + \frac{1}{2}), \tag{4}$$

where $\mathcal{N}$ is the operator number, ω_i is the frequency of the oscillator and $\hbar = h/2\pi$ (h is the Planck constant). The partition function can be found by standard methods; the free energy takes the form

$$F^{Phonon} = \frac{1}{2}\hbar \sum_{i=1}^{N} \omega_i + k_B T \sum_{i=1}^{N} \log(1 - e^{\hbar\omega_i/k_B T}). \tag{5}$$

Since there is a finite number of particles there will be a superior bound for the possible number of modes for the particles,

$$N = \left(\frac{\ell}{2\pi}\right)^D \frac{\pi^{D/2}}{\Gamma(D/2+1)} k_c^D, \tag{6}$$

where k_c will be the maximum-k-mode. Let us consider ^{4}He as a continuous medium and assume the anomalous dispersion relation for phonons $w = c_o k(1 - \alpha k^2)$, where c_o is the sound velocity, and $\alpha < 0$ as it has been experimentally estimated [1, 2] and theoretically justified [4]. For a large number of particles N, we can replace all summations by integrations; then Eq.(5) can be written as

$$F^{Phonon} = F_o + N k_B T \log\left(1 - e^{-\frac{\theta}{T}(1-\alpha k_c^2)}\right) - \frac{N k_B}{\theta^D} T^{D+1} \int_0^{\theta/T} dx x^D \frac{(1 - 3t^2x^2)}{\exp(x(1-t^2x^2)) - 1}, \tag{7}$$

where $\theta = \hbar c_o k_c / k_B$, $t = \sqrt{\alpha}\;\; k_c T/\theta$ and

$$F_o = \frac{1}{2} N k_B \theta \left(\frac{1}{D+1} - \frac{1}{D+3}\alpha k_c^2\right).$$

It is possible to find the internal energy $U^{Phonon} = F^{Phonon} - T\partial F^{Phonon}/\partial T$; thus we get

$$U^{Phonon} = U_o + D\frac{N k_B}{\theta^D} T^{D+1} \int_0^{\theta/T} dx x^D \frac{(1 - t^2x^2)}{\exp(x(1-t^2x^2)) - 1}, \tag{8}$$

with $U_o = F_o$, and the specific heat at constant volume can be obtained from $C^{Phonon} = (\partial U^{Phonon}/\partial T)_V$.

We take for the energy of the roton gas its usual dispersion relation $\epsilon = \Delta + (p - p_o)^2/2\mu$, where p_o is the momentum value for the energy minimum and μ is the effective mass of the roton. Using standard methods we obtain the free energy in D dimensions:

$$F^{Roton} = R^{(D)} \left(\frac{\Delta}{k_B}\right) \left(\frac{k_B T}{\Delta}\right)^{3/2} \exp(-\Delta/k_B T). \tag{9}$$

The corresponding internal energy is given by

$$U^{Roton} = R^{(D)} \left(\frac{\Delta}{k_B}\right) \left[\left(\frac{\Delta}{k_B T}\right)^{1/2} + \frac{1}{2} \left(\frac{\Delta}{k_B T}\right)^{3/2} \right] \exp(-\Delta/k_B T), \tag{10}$$

and the specific heat can be written as

$$C^{Roton} = R^{(D)} \left[\frac{3}{4} \left(\frac{k_B T}{\Delta}\right)^{1/2} + \left(\frac{\Delta}{k_B T}\right)^{1/2} + \left(\frac{\Delta}{k_B T}\right)^{3/2} \right] \exp(-\Delta/k_B T) \tag{11}$$

where

$$R^{(D)} = \left(\frac{\ell}{2\pi\hbar}\right)^D \frac{2\pi^{D/2}}{\Gamma(D/2)} p_o^{D-1} \sqrt{2\pi\mu\Delta} \ \ k_B$$

In general, the additive properties of the Boltzmann-Gibss statistics give $F_{BG} = F^{Phonon} + F^{Roton}$ for the free energy (in its extended form it is called the fundamental equation for the system), $U_{BG} = U^{Phonon} + U^{Roton}$ for the internal energy and $C_{BG} = C^{Phonon} + C^{Roton}$ for the specific heat.

As an alternative, we present a calculation within the Tsallis generalized statistics. This kind of calculation is useful when the system is expected to violate the extensive properties. More precisely [8], the difficulties and their consequences are classified as follows:

(i) For a relevant euclidean-like (non-fractal) space-time and if either the forces or the memory (or both) are long-ranged but we are interested in an equilibrium state, the Boltzmann-Gibbs statistics is weakly violated and the formalism can be used to obtain an approximate description. However, if we are interested in a meta-equilibrium state, the Boltzmann-Gibbs description is strongly violated. Another formalism must be used.

(ii) For a relevant (multi)fractal space, the Boltzmann-Gibbs formalism is strongly violated once more and another formalism is needed.

The explicit need for a non-extensive thermodynamics has been well known from cosmology, gravitation and astrophysics [9], magnetic systems [10], Lévy-like anomalous diffusion [11], etc. Consequently, Tsallis proposed a non-extensive thermostatistics in [6]. This formalism has already received some applications. Among them, let us mention the following ones: self-gravitating systems, stellar polytropes, Vlasov equation [12, 13]; Lévy-like anomalous diffusion [11, 14] and correlated anomalous diffusion [8, 15]. Furthermore, its connection with quantum statistics [16], quantum uncertainty [17], fractals [18, 19], dynamical linear response theory [20], etc., has been established. The specific heat of some simple systems has been studied; among them we have: confined free particle [21], anisotropic rigid rotator [22], hydrogen atom [23], etc.

Tsallis' generalized statistics relies on entropy

$$S_T \equiv -k\frac{1-\sum_R p_R^{q_T}}{1-q_T}, \tag{12}$$

where $q_T \in \Re$; k is a positive constant and S_T recovers the standard form $-k_B\sum_R p_R \ln p_R$, in the limit $q_T \to 1$.

Expression (12) has enabled several (nontrivial, although mathematically simple and natural) generalizations of important properties (see, for example ref. [21] for canonical ensemble calculations and ref. [16] for grand-canonical ones).

(i) The generalized canonical distribution adopts the form

$$p_R = \frac{[1-\beta(1-q_T)\varepsilon_R]^{\frac{1}{1-q_T}}}{Z_T}, \tag{13}$$

with the generalized partition function consistently given by

$$Z_T(\beta) = \sum_R [1-\beta(1-q_T)\varepsilon_R]^{\frac{1}{1-q_T}}\ , \tag{14}$$

where $\beta \equiv 1/kT > 0$ and ε_R is the spectrum (R represents a set of given real numbers).

(ii) The thermodynamics associated with Eq.(12) is invariant under Legendre transformations and preserves thermodynamic stability [24]; in particular, the fundamental equation is

$$F_T = -kT\frac{Z_T^{1-q_T}-1}{1-q_T}. \tag{15}$$

The q_T-expectation value of the energy is given by $U_T = \sum_R p_R^{q_T}\varepsilon_R = F_T - T(\partial F_T/\partial T)$ and the generalized specific heat is $C_T = \partial U_T/\partial T$.

Due to the small departure from the Boltzmann-Gibbs result and to the mathematical difficulties associated with a generic value of q_T , let us focus from now on the $q_T \approx 1$ case. Similar approximations were applied in precedent works [25, 26]. By using Eq.(7) from ref. [25], the generalized specific heat (C_T) asymptotically becomes

$$\begin{aligned} C_T \ \approx\ & \exp\left(-(1-q_T)F_{BG}/k_BT\right)\times \\ & \left[C_{BG} + \frac{1-q_T}{k_B}\left(2U_{BG}\frac{C_{BG}}{T} - C_{BG}^2 - U_{BG}\frac{\partial C_{BG}}{\partial T} - k_BT\frac{\partial C_{BG}}{\partial T} - \frac{1}{2}k_BT^2\frac{\partial^2 C_{BG}}{\partial T^2}\right)\right]. \end{aligned} \tag{16}$$

For the following calculation we take $D = 3$, $N_A(1-q_T) \approx 10^{-2}$, where N_A is the Avogadro number and we use the data for sample 6 measured by Greywall [2], thus, $\ell^3 = 27.579\ cm^3$ is the molar volume, $\Delta/k_B = 8.72$, $R^{(3)} = 6.19\times 10^4$ and $c_o = 237m/s$.

In FIG.2., we show the profile of the experimental data of the specific heat (dashed line) and its generalized form according to Eq.(16) and, as we can see, the results seem to be good. For $T \to 0$ we have $C_T > C_E$, but as T increases there is a temperature at which C_T equals C_E; for temperatures higher than this value $C_T < C_E$. We have chosen sample 6 of ref. [2] in order to compare our results with those of ref. [4].

If we compare carefully the results from quantum groups, Boltzmann-Gibbs and Tsallis thermostatistics with the experimental data, we find a rather interesting result. Indeed, although we do not have a microscopic model for excitations in ^{4}He and are just applying statistical methods, comparison with experimental data do not show substantial differences between our results and those of quantum groups [4] and Boltzmann-Gibbs statistics. In FIG.3., the relative difference of each known expression to the values of C_E measured by Greywall is depicted.

We see that for small values of T, i.e., when the particles interact weakly, the Boltzmann-Gibbs statistics is better. As T increases, interactions become important and, consequently, C_{BG} differs more from C_E, while C_T and C_{QG} are closer to experimental values.

Summarizing, all the available theories are of the same order of accuracy and, if a better theoretical approach to the liquid ^{4}He specific heat is to be obtained, a theory is needed that considers phonon-phonon, roton-roton and phonon-roton interactions in the Hamiltonian.

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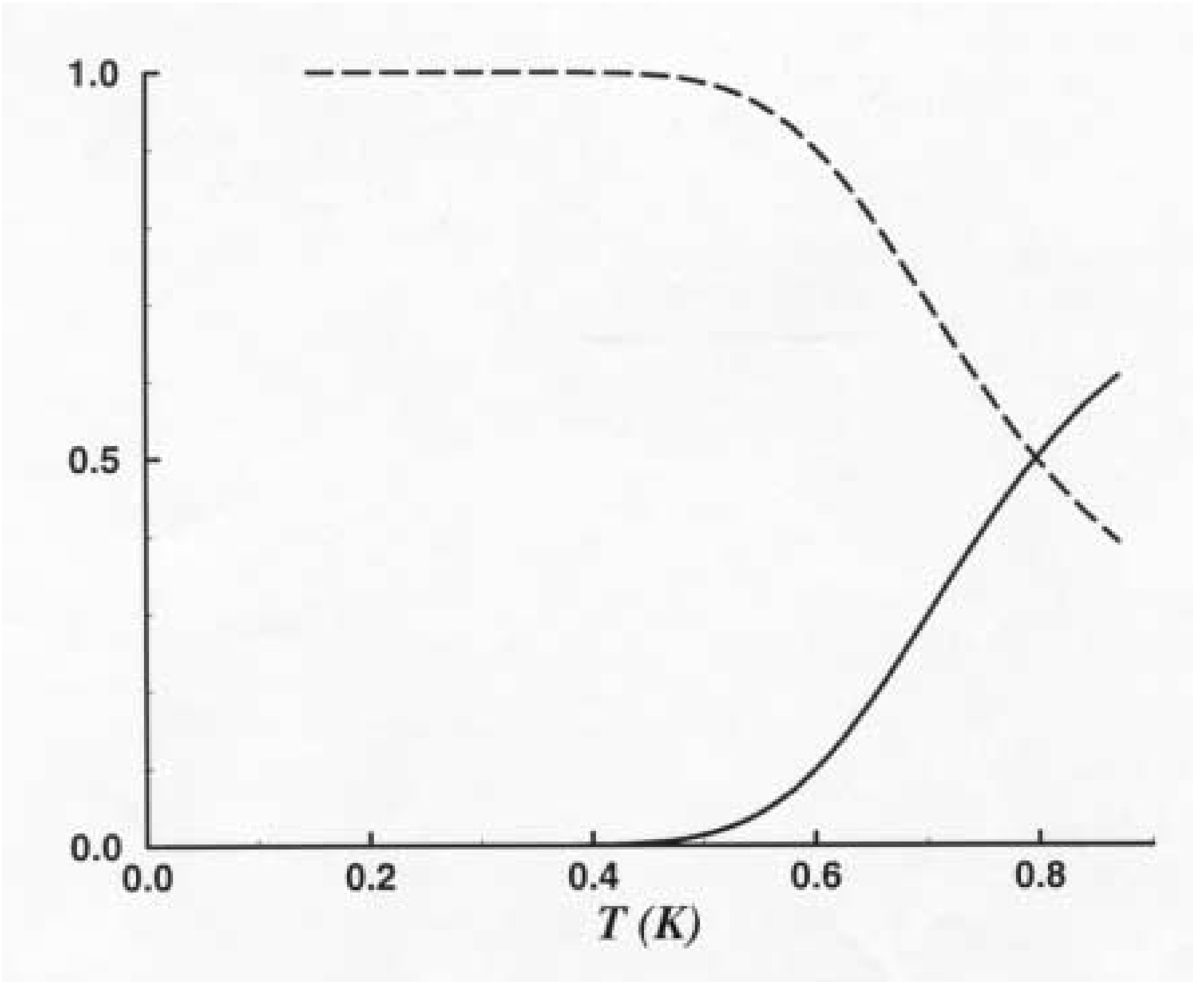

FIG.1. Relative phonon (dashed line; C_E^{Phonon}/C_E) and roton (solid line; C_E^{Roton}/C_E) contributions to the specific heat of ^{4}He.

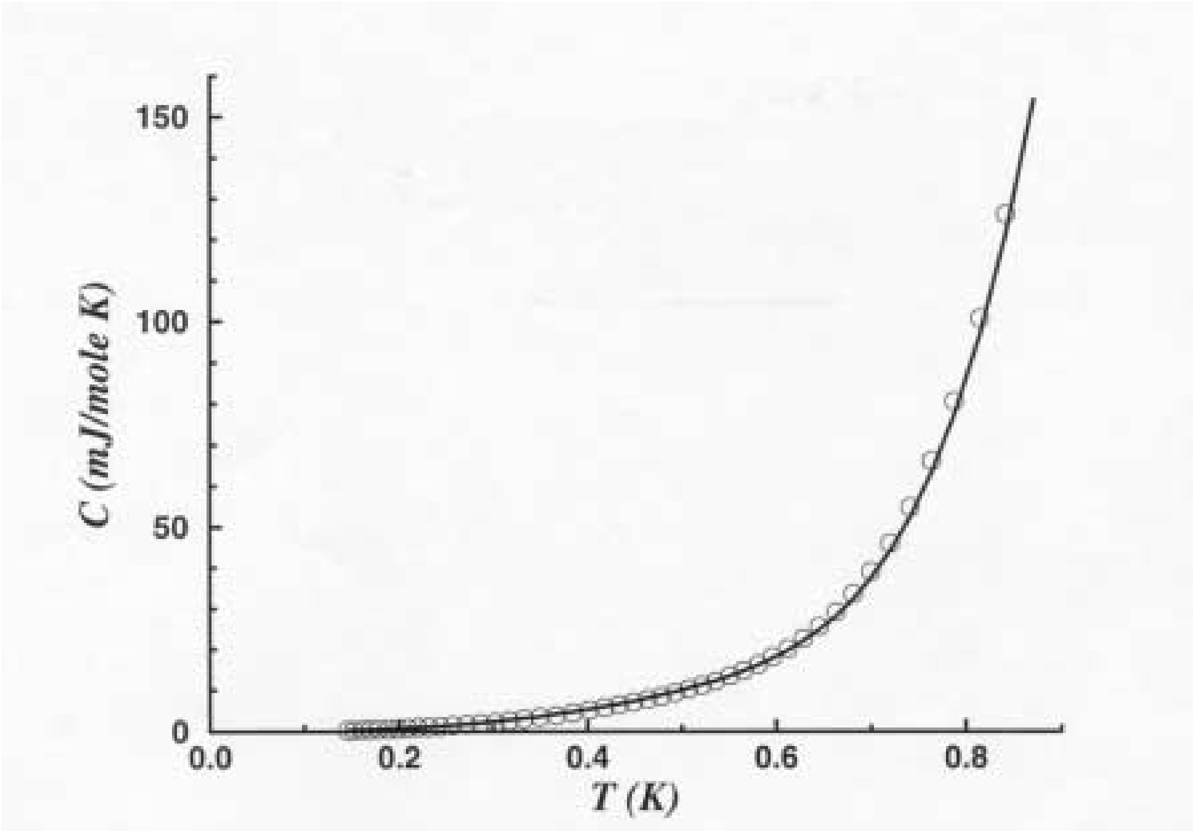

FIG.2. Experimental (dashed line; $C \equiv C_E$) and present theoretical (solid line; $C \equiv C_T$) curves for the specific heat of ^{4}He. Experimental values correspond to sample 6 of ref. [2] as it was made in ref. [4]. Theoretical values were computed from Eq.(16). We have used the data measured by Greywall.

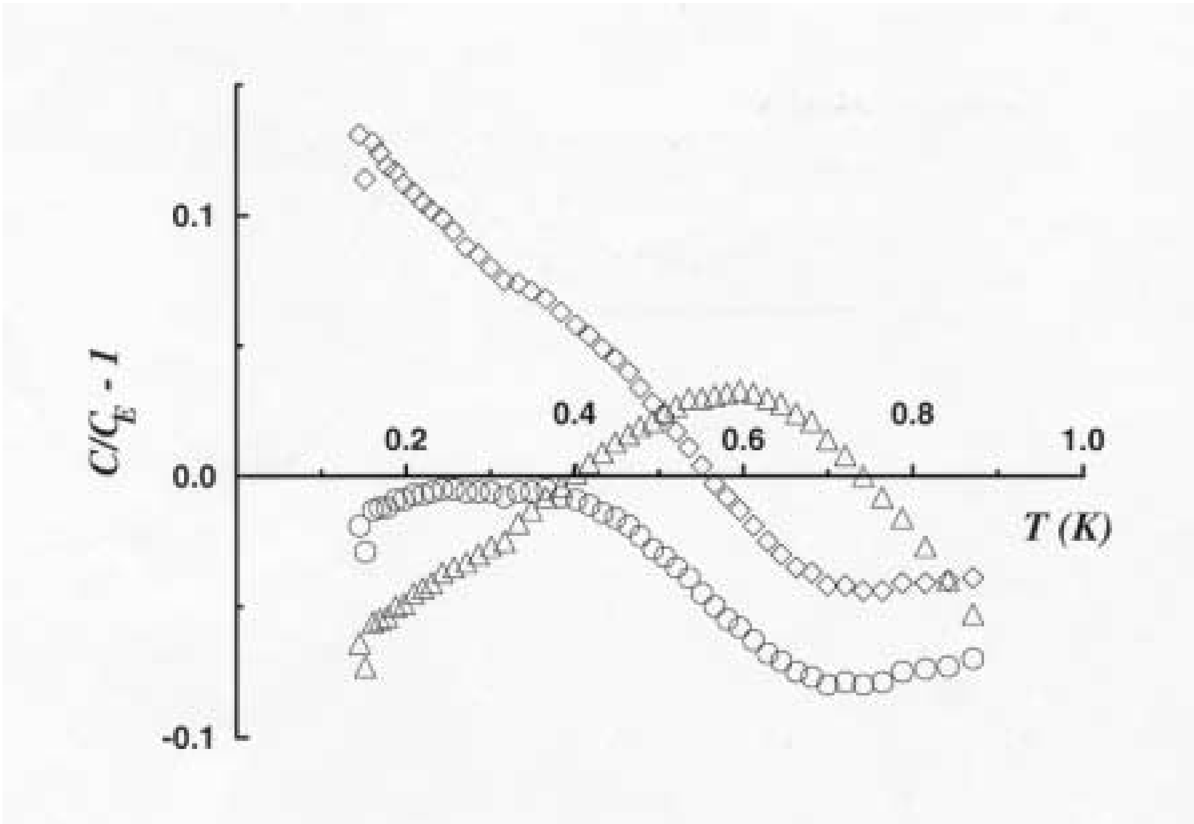

FIG.3. Relative difference between experimental data (sample 6 of reference [2] as in ref. [4]; C_E) and the different theories; Boltzmann-Gibbs (circles ; $C \equiv C_{BG}$), quantum groups (triangles; $C \equiv C_{QG}$) and Tsallis thermostatistics (diamonds; $C \equiv C_T$). We have also used the data measured by Greywall.

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