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SPECIFIC HEAT OF THE HARMONIC OSCILLATOR WITHIN GENERALIZED EQUILIBRIUM STATISTICS

by

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Abstract

Within the generalized equilibrium statistics recently introduced by Tsallis ($p_n \propto [1-\beta(q-1)\epsilon_n]^{1/(q-1)}$), we calculate the thermal dependence of the specific heat corresponding to a harmonic-oscillator-like spectrum, namely, $\epsilon_n = \omega(n-\alpha)$, ($\forall\omega > 0$, $n = 0, 1, 2, \ldots$). The influences of q and α are exhibited. Physically inaccessible and/or thermally frozen gaps are obtained in the low temperature region, and, for $q > 1$, oscillations are observed in the high temperature region. The specific heat of the two-level system is also shown.

Key-words

generalized equilibrium statistics, harmonic oscillator, multifractals, two-level system

Recently a generalization of Boltzmann-Gibbs (BG) equilibrium statistics has been proposed by Tsallis[1]. This distribution is based on a generalized definition of entropy as follows[1]:

$$S_q = k\frac{1-\sum_n p_n^q}{q-1}, \tag{1}$$

where p_n, q and k denote the emergence probability of state n, a real number which characterizes the statistics and a universal constant, respectively. The $q \to 1$ limit corresponds to the standard entropy, namely,

$$S = -k\sum_n p_n \log p_n. \tag{2}$$

The canonical distribution is derived by extremizing entropy (1) (or, equivalently, by extremizing the Renyi entropy[1,2]) under the condition that the average "energy "is constant. The emergence probability p_n of state n with "energy"ϵ_n is proportional to

$$\{1-\beta(q-1)\epsilon_n\}^{\frac{1}{q-1}}. \tag{3}$$

Therefore

$$p_n = \frac{1}{Z_q}\{1-\beta(q-1)\epsilon_n\}^{\frac{1}{q-1}}, \tag{4}$$

where

$$Z_q = \sum_n \{1-\beta(q-1)\epsilon_n\}^{\frac{1}{q-1}}. \tag{5}$$

β is a Lagrange parameter which is interpreted as an inverse "temperature", that is, $\beta = 1/kT$. If the condition

$$1-\beta(q-1)\epsilon_n > 0 \tag{6}$$

does not hold, for some state, its associated probability is defined to be zero and consequently the summation in eq.(5) runs only over the states which satisfy the condition (6). If no state satisfies this condition, we call such parameter region *unphysical* or *physically inaccessible*. If only one state satisfies the condition (6), we call such region *thermally frozen*. In the $q \to 1$ limit, expression (3) reproduces the BG result, namely, $p_n \propto \exp(-\beta\epsilon_n)$.

Under this distribution, we will consider the thermodynamic quantities of some systems. The "internal energy"U is in general given by

$$U = <\epsilon_n> \equiv \sum_n p_n \epsilon_n, \tag{7}$$

where $<\cdots>$ denotes the average under the distribution (4). Hence the "specific heat"C is given by

$$\begin{aligned} C &\equiv \frac{\partial U}{\partial T} = -k\beta^2\frac{\partial U}{\partial \beta} \\ &= k\beta^2\{<\frac{\epsilon^2}{1-\beta(q-1)\epsilon_n}> - U < \frac{\epsilon_n}{1-\beta(q-1)\epsilon_n}>\}. \end{aligned} \tag{8}$$

The simplest system, namely a non-degenerate two-level one ($\epsilon_n = \omega(n-\alpha), n = 0,1$ and $\forall\omega > 0$), has been discussed in Ref.[1], where its internal energy $U(T)$ was explicitly obtained. For future comparison, let us just calculate here, and present in Fig.1, the corresponding specific heat C.

Let us then calculate the specific heat C associated with another very elementary system, namely a harmonic-oscillator-like one, characterized by the spectrum

$$\epsilon_n = \omega(n-\alpha) \tag{9}$$

with $\omega > 0$, $\alpha \in \mathbf{R}$ and $n = 0,1,2,\ldots$.

The behavior of distribution p_n for large value of n and $q < 1$ is given by

$$p_n \sim n^{\frac{1}{q-1}} \quad (n \to \infty). \tag{10}$$

Hence some momenta of this distribution are divergent. The partition function diverges for $1/(q-1) > -1$, that is, $q < 0$. The internal energy diverges for $1/(q-1)+1 > -1$, that is, $q < 1/2$. The specific heat diverges for $1/(q-1)+2 > -1$, that is, $q < 2/3$. These divergences are of the order of $\zeta(s)$ with $s \to 1+0$, where $\zeta(s)$ is the Riemann's zeta function:

$$\zeta(s) = \sum_{k=1}^{\infty} \frac{1}{k^s} \tag{11}$$

and $s = m + 1/(q-1)$ where m is an integer which is characteristic of the quantity we are considering. We have performed computer calculations of the specific heat. The results are presented in Fig.2. We remark that:

(i) In the $kT/\omega \to \infty$ limit, C/k attains an α-independent value which equals 1 for $q = 1$, and monotonously decreases from infinity to zero when q increases from $2/3$ to infinity.

(ii) For $q > 1$ (and only then), C presents, in the high temperature region, oscillations whose thermal period is $k\Delta T/\omega = q-1$, the minima (maxima) of the oscillations are cusp- like (rounded).

(iii) For $2/3 < q \leq 1$ and all values of α, C vanishes with vanishing temperature.

(iv) The frozen and inaccessible regions are summarized in what follows:

For $\alpha > 1$, there is neither frozen nor inaccessible regions.

For $1 \geq \alpha > 0$, there is no inaccessible region and the frozen region is given by

$$0 < \frac{kT}{\omega} \leq (1-\alpha)(q-1) \text{ if } q > 1,$$

and by

$$0 > \frac{kT}{\omega} \geq (1-\alpha)(q-1) \text{ if } q < 1.$$

For $\alpha \leq 0$: if $q > 1$,

$$0 < \frac{kT}{\omega} \leq -\alpha(q-1) \text{ corresponds to an inaccessible region}$$

and

$$-\alpha(q-1) < \frac{kT}{\omega} \leq (1-\alpha)(q-1) \text{ corresponds to a frozen one;}$$

if $q < 1$,

$$0 > \frac{kT}{\omega} \geq -\alpha(q-1) \text{ corresponds to an inaccessible region}$$

and

$$-\alpha(q-1) > \frac{kT}{\omega} \geq (1-\alpha)(q-1) \text{ corresponds to a frozen one.}$$

(v) For $q = 2$ ($q > 2$) and all values of α, C discontinuously jumps from zero to a finite (or infinite) value in the low temperature region, similarly to what occurs in the two-level system.

As a final remark let us recall[1] that for the present generalized statistics physical applications are still to be identified. One can speculate on some candidates for applications, for example, multifractals, nonergodic systems where non-euclidean occupation of the phase space might occur, quantum gravity or similar situations with fluctuating metrics. The specific heat remarkable properties herein exhibited (mainly the oscillations and the existence of forbidden and frozen gaps) might be very helpful for identifying such applications.

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References

[1] C.Tsallis, J. Stat. Phys. **52** (1988) 497.

[2] A.Renyi, Probability Theory (North-Holland, 1970).

Figure Captions

Figure 1 Thermal dependence of the specific heat of the two-level system:
(a) $\alpha = -1/2$ (the curves are invariant under $q-1 \leftrightarrow 1-q$);
(b) $q = 2$ (the curves are invariant under $[kT/\omega, (1/2-\alpha)] \leftrightarrow [-kT/\omega, -(1/2-\alpha)]$).

Figure 2 Thermal dependence of the specific heat of the harmonic oscillator:
(a) $\alpha = 0$;
(b) typical values of q and α.

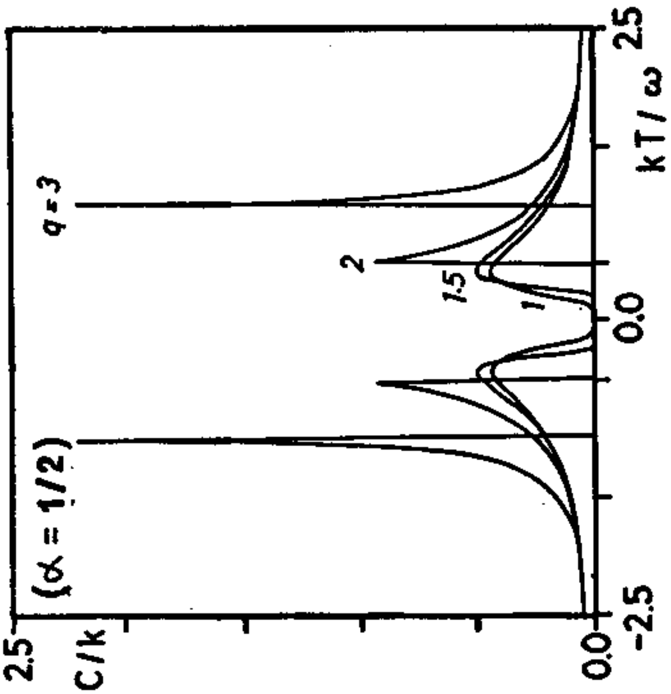

FIG. 1(a)

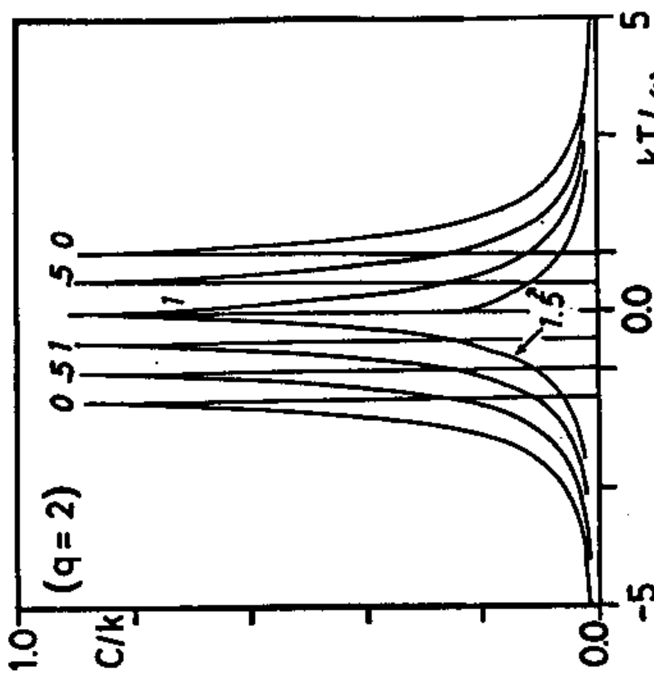

FIG. 1(b)

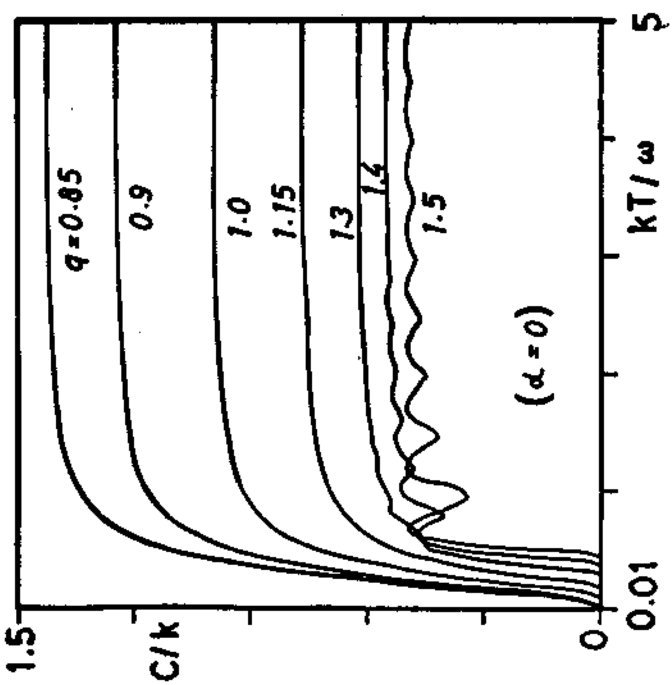
1.5
C/k
0
0.01
5
kT/ω
q=0.85
0.9
1.0
1.15
1.3
1.4
1.5
(α=0)

FIG. 2(a)

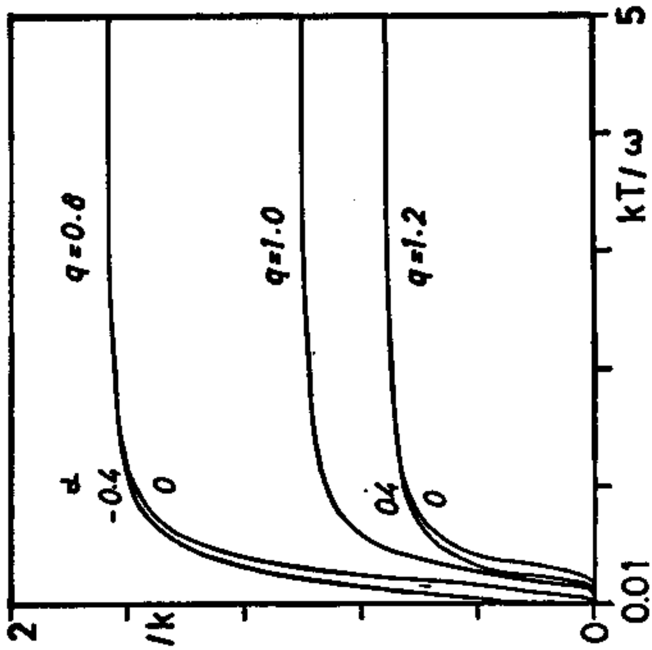
2
C/k
0
0.01
5
kT/ω
q=0.8
q=1.0
q=1.2
α
-0.4
0
0.4
0

FIG. 2(b)