

Phase Space Cell in Nonextensive Classical Systems

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Received: 25 July 2002 / Accepted: 31 March 2003 / Published: 30 June 2003

Abstract: We calculate the phase space volume Ω occupied by a nonextensive system of N classical particles described by an equilibrium (or steady-state, or long-term stationary state of a nonequilibrium system) distribution function, which slightly deviates from Maxwell-Boltzmann (MB) distribution in the high energy tail. We explicitly require that the number of accessible microstates does not change respect to the extensive MB case. We also derive, within a classical scheme, an analytical expression of the elementary cell that can be seen as a macrocell, different from the third power of Planck constant. Thermodynamic quantities like entropy, chemical potential and free energy of a classical ideal gas, depending on elementary cell, are evaluated. Considering the fractional deviation from MB distribution we can deduce a physical meaning of the nonextensive parameter q of the Tsallis nonextensive thermostatistics in terms of particle correlation functions (valid at least in the case, discussed in this work, of small deviations from MB standard case).

PACS numbers: 05.20.-y, 05.70.-a

Keywords: Classical Statistical Mechanics, Thermodynamics.

1. Introduction

Statistical description of a system of N particles requires the subdivision of the phase space into equidimensional elementary cells of phase volume $\Delta\Omega$, which can be determined by the laws of nature (comparison with quantum evaluation of energy state density) and experimentally measured, for instance, in the low temperature heat capacity of a crystal or in the Stefan-Boltzmann constant.

In the phase space volume of a system of particles described by quantum distribution the smallest elementary cell is the third power of the Planck constant. For classical particles the elementary cell is, in principle, undetermined. This is true particularly in the limiting case of small occupation numbers (when MB distribution is valid) and the phase space volume of a cell acquires arbitrary values. The problem of dividing the phase space into finite cells was solved when a natural way to derive dimension of elementary cells within MB statistics using energy quantization was found. However, quantum discontinuity can be lost when dimension of the volume containing the gas increases and the quantum states become even and even more numerous [1]. Only the insertion of the Pauli exclusion principle enables us to solve this problem.

Boltzmann's request of a great number of particles into the cell is usually not verified (one particle every 30000 cells in normal conditions)[2]. However, if the number is small, it is possible to combine many cells and form a greater cell (macrocell) containing more particles [3].

This paper aims at examining first of all how, in the nonextensive thermostatics (NETS), the elementary cell differs from the one of the extensive MB case, requiring explicitly that the number of accessible microstates be the same in both (extensive and nonextensive) phase spaces and obtain also, within a classical scheme and without quantum arguments, explicit expressions of the cells. Let us briefly recall that NETS has been developed in the last years mainly after the works of Tsallis [4, 5] which introduced a generalized entropy, featured by an entropic parameter q , whose meaning is not fully understood yet (more generally, it can be defined in terms of fluctuations of intensive quantities like temperature [6–8]; explicit analytical expressions of q in terms of physical quantities exist in few cases, like, for instance, in turbulence problems [9] and in the description of solar plasma [10, 11]).

The value of q is not easily given a priori for a given particular system, without comparing calculations to available experimental results. The NETS is now applied to a great variety of problems, from genetics and biology to astrophysics (see ref.s [12] and [13] for a complete list of basic works and applications).

The approach to NETS we are showing in this paper, is based on the analysis of deviations from standard phase space volume and on a new definition of elementary cell. This new approach will probably provide, in the near future, a better understanding of the meaning of the parameter q . The validity of our treatment can be extended to statistics different from the Tsallis version of NETS, when complete deformed distribution functions are considered, and to large deviations from MB phase space volume.

In Section 2, by comparing the number of allowed microstates W_0 in the MB extensive phase space Ω_0 and in the deformed phase space Ω , we derive the dimensions of both elementary cells $\Delta\Omega_0$ and

$\Delta\Omega$. The cell $\Delta\Omega$ results to be smaller than $\Delta\Omega_0$ (if $q < 1$) so that, in this case, the third power of Planck constant is not suitable as the value of $\Delta\Omega_0$ because h^3 is the smallest cell admissible due to the Heisenberg principle. Otherwise $\Delta\Omega$ is larger than, $\Delta\Omega_0$ if $q > 1$ (h is expressed in units [energy length]).

By considering the nonextensive Tsallis equilibrium (or steady state, or long-term stationary state of a nonequilibrium system) distribution, we limit ourselves to small deviations, with the absolute value of the parameter $\delta = (1 - q)/2$ much smaller than one (we recall that for $q \rightarrow 1$ all the MB results must be recovered).

We must realize that deviations, although small, are not negligible in those energy islands of Ω where quantities like, for instance, nuclear reaction rates, rates of atomic processes and of chemical reactions, electron transport in semiconductors are very sensible to them [10, 14–16]. In Section 3, we discuss the case of nonextensive classical ideal gas. We compare our results with those recently derived by several authors, among them see ref.s [17–19], and we calculate the entropy, the chemical potential and free energy discussing the results. We deduce also in Section 4 an interpretation of the parameter q using the calculated phase volume Ω as a function of fractional deviation, occupied by a nonextensive system of N classical particles. The physical meaning is derived in terms of particle correlation function. Conclusions are reported in Section 5.

2. Phase Space Volume and Elementary Cell

The state of a system of N particles is specified in the $6N$ dimensional phase space (Γ space). Its volume $\Omega[n_r]$ can be divided into small cells of volume $\Delta\Omega$, so that coordinates do not vary sensibly within them.

The volume contains the N particles distributed in a certain set of numbers $(n_1, n_2, \dots, n_t) = [n_r]$ and is given by:

$$\Omega[n_r] = \frac{N!}{n_1!n_2!\dots n_t!} (\Delta\Omega)^N. \quad (2.1)$$

The number of accessible microstates is defined (including the factor $1/N!$) by [20]

$$W = \frac{\Omega}{N!(\Delta\Omega)^N}. \quad (2.2)$$

It is well known that $\ln \Omega$ can be represented through the Stirling approximation

$$\ln \Omega \approx N \ln N + N \ln \Delta\Omega - \sum_i n_i \ln n_i. \quad (2.3)$$

Having Ω a maximum, its logarithm can be expanded in a series of powers of $\partial n_i = n_i - n_{i_0}$, where n_{i_0} is the distribution function for which Ω has a maximum, indicated by Ω_0 (the symbol ∂ means variation). After using the Lagrange method with the usual constraints and with negligible interactions the following is obtained:

$$n_{i_0} = A_M e^{-x_i}, \quad \sum_i n_{i_0} = N, \quad \sum_i n_{i_0} x_i = \frac{3}{2} N,$$

$$x_i = \beta \epsilon_i, \quad \beta = \frac{1}{kT}, \tag{2.4}$$

$$A_M = \frac{N}{V} \left(\frac{\beta}{2 \pi m} \right)^{3/2} \Delta\Omega_0.$$

The mass of the particles m is in energy units. The number of accessible microstates in Ω_0 is of course

$$W_0 = \frac{\Omega_0}{N! (\Delta\Omega_0)^N}, \tag{2.5}$$

(let consider the following example: for a classical ideal gas, if N is large we have that $W_0 = e^N / \sqrt{2 \pi N}$ see Section 3).

We are now interested in the volume in the Γ space corresponding to a NETS distribution having small deviations from the MB distribution. The deviations in the high energy tail are particularly interesting. Following the approach to general statistical problem in physics by Bohm and Schützer [21] after expanding up to the second power in ∂n_i the Lagrange equation, alternative definition of Ω is obtained:

$$\ln \Omega = \ln \Omega_0 - \frac{1}{2} \sum_i \frac{(\partial n_i)^2}{n_{i_0}}, \tag{2.6}$$

or

$$\Omega = \Omega_0 \exp \left[-\frac{1}{2} \sum_i n_{i_0} (\partial f_i)^2 \right], \tag{2.7}$$

with the fractional deviation from MB distribution given by

$$\partial f_i = \frac{\partial n_i}{n_{i_0}}. \tag{2.8}$$

Let us introduce the non-Maxwellian distribution

$$n_i = A_T A_\delta \exp(-y_i - \delta y_i^2). \tag{2.9}$$

Eq.(2.9) represents a distribution, mainly differing from Maxwellian in the high energy tail, depending on the sign of δ [$\delta > 0$, ($q < 1$): depleted tail; $\delta < 0$, ($q > 1$): enhanced tail]; it can be derived, for instance, from the Tsallis distribution

$$n_T = Z_q(\beta^*)^{-1} \left[1 - (1-q)\beta^* \left(\sum_i \frac{p_i^2}{2m} - U_q \right) \right]^{\frac{1}{1-q}}, \tag{2.10}$$

when deviations from MB distribution are small, $Z_q(\beta^*)$ is the generalized partition function and U_q the internal energy. Eq. (2.9) may represent an equilibrium distribution or a steady state, or a long-term stationary state of a nonequilibrium system. In Eq. (2.9)

$$A_T = \frac{N}{V} \left(\frac{\beta^*}{2 \pi m} \right)^{3/2} \Delta\Omega. \tag{2.11}$$

$\Delta\Omega$ is the deformed elementary cell of the phase space Ω , β^* is the Lagrange multiplier of the phase space Ω , different from β (the Lagrange multiplier in Ω_0), defined below in (2.24).

We also have

$$A_\delta = 1 + \frac{15}{4} \delta - 30\delta^2, \tag{2.12}$$

$$y_i = \beta^* \epsilon_i. \tag{2.13}$$

ϵ_i are the energies of the different microstates with the same values of those of the phase space Ω_0 .

The constraints are

$$\sum_i n_i = N, \quad \sum_i n_i y_i = \frac{3}{2} N, \tag{2.14}$$

where the second one is the energy NETS average value when deviations are small. Other distributions, based on other statistics can be used [22, 23]; of course, when deformations are small, these distributions can be fitted with good approximation by Eq. (2.9). The use of exact distributions, derived from other generalized statistics is possible at least numerically; in this work, however, we limit ourselves to consider only the distribution of Eq. (2.9), in order to simplify the question.

The volumes Ω_0 and Ω are different in size. $\Delta\Omega_0$ and $\Delta\Omega$ are also different. We realize that the differences could be considered negligible, while their effects seem to be quite important for the evaluation of several physical quantities. Let us remark that the number of microstates or discrete events does not change from one space to the other one. Therefore, we set the equation $W = W_0$, because we want to count the same number of microstates both in Ω and Ω_0 . Using the relations reported above in this Section, we can explicitate the expressions of Ω and $\Delta\Omega$ after simple calculations. After using the following relations:

$$\frac{A_T}{A_M} = \frac{\Delta\Omega}{\Delta\Omega_0} \left(\frac{\beta^*}{\beta} \right)^{3/2} = \frac{e^{9\delta/4}}{A_\delta}, \tag{2.15}$$

$$\frac{A_\delta^2}{A_{2\delta}} = 1 + \frac{1185}{16} \delta^2, \tag{2.16}$$

$$\sum_i \frac{n_i^2}{n_{i_0}} = N \left(1 + 18 \delta - \frac{3799}{32} \delta^2 \right), \tag{2.17}$$

noting that the explicit calculation of (2.17) requires the evaluation of the average value

$$\left\langle \frac{e^{-x_i}}{e^{-y_i}} \right\rangle \approx \exp \left(\frac{37}{2} \delta - \frac{11841}{64} \delta^2 \right), \tag{2.18}$$

finally, we obtain Ω and $\Delta\Omega$ as functions of Ω_0 and $\Delta\Omega_0$, respectively as follows:

$$\frac{\Omega}{\Omega_0} = \exp \left[-\frac{1}{2} N \left(\frac{1}{N} \sum_i \frac{n_i^2}{n_{i_0}} - 1 \right) \right] = \exp \left[-\frac{1}{2} N \left(18 \delta - \frac{3799}{32} \delta^2 \right) \right], \tag{2.19}$$

$$\frac{\Delta\Omega}{\Delta\Omega_0} = \exp \left[-\frac{1}{2} \left(18 \delta - \frac{3799}{32} \delta^2 \right) \right]. \tag{2.20}$$

The systems featured by $\Delta > 0$ ($q < 1$) have $\Delta\Omega$ smaller than $\Delta\Omega_0$. Therefore, we are not allowed in their classical extensive description to take $\Delta\Omega_0 = h^3$, because h^3 should be the smallest elementary

permissible cell. On the other hand, we shall verify that $\Delta\Omega_0$ must always be much larger than h^3 . It must be a macrocell. The equation of state calculated by means of the distribution (2.9) is given by

$$PV = NkTC_\delta = NC_\delta / \beta, \tag{2.21}$$

where

$$C_\delta = 1 - 5\delta + 46\delta^2, \tag{2.22}$$

Let us anticipate that for a nonextensive classical ideal gas after exact calculations with the exact distribution (2.10), one can obtain the following relation, at any value of q [17, 18]

$$PV = N\beta^* = NC_q / \beta, \tag{2.23}$$

$$\beta^* C_q = \beta, \tag{2.24}$$

where $C_q = Zq(\beta)^{1-q}$.

We compare (2.21) and (2.22) to (2.23) and (2.24) in the case of small deviations. With the condition $3N(1-q)/2 = 3N\delta > 1$ the quantity C_q reduces to C_δ if we assume an elementary cell given by

$$\Delta\Omega = \left(\frac{2\pi m}{\beta}\right)^{3/2} \frac{V}{N}, \tag{2.25}$$

and we recover the correct formal expression of the equation of state reported in Eq. (2.21). This value of Ω_0 imposes that

$$A_M = 1, \quad \text{and} \quad A_T = 1 - \frac{3}{2}\delta + \frac{1221}{32}\delta^2. \tag{2.26}$$

Therefore, the requirements that $W = W_0$ and that the equation of state for NETS classical systems be correctly expressed also in the small deviations limit imply that the standard phase space elementary cell be given by the expression (2.25) (we send to Sect. 3 for some more details).

This elementary cell can indeed be considered a macrocell, particularly if compared to the value of h^3 , usually taken as elementary cell. However, this requirement is not a problem, because of the uncertainty of the classical elementary cell and because Darwin and Fowler [3] showed that macrocells should be used to satisfy Boltzmann requirements of a great average number of particles in each cell.

To take $\Delta\Omega_0$ of Eq. (2.25) means to have one particle in each macrocell and, posing $\Delta\Omega_0 = Xh^3$, to have $1/X$ particles in each microcell h^3 , i.e. one particle in thousands of cells, where

$$X = \left(\frac{2\pi m}{\beta}\right)^{3/2} \frac{V}{N h^3}, \tag{2.27}$$

which is not a pure number, but depends on β . The elementary cell in the deformed phase space is from (2.20)

$$\Delta\Omega = \left(\frac{2\pi m}{\beta^*}\right)^{3/2} \frac{V}{N} = \left(\frac{2\pi m}{\beta}\right)^{3/2} \frac{V}{N} C_\delta^{3/2}, \tag{2.28}$$

which is a macrocell. We can write $\Delta\Omega = Yh^3$, each macrocell containing one of the N particles, where

$$Y = \left(\frac{2\pi m}{\beta}\right)^{3/2} \frac{V}{N} \frac{C_\delta^{3/2}}{h^3},$$

is a quantity depending on β and q or on β^* . The subdivision of the phase space volume Ω in microcells equal to h^3 does not allow the conservation of the value of the number of permissible microstates, nor the subdivision in a fixed number of micro cells independent on β and q .

Instead of having an elementary cell which does not depend on the Lagrange multiplier β and is the third power of a universal constant (Planck constant) and the number of elementary cells forming the total phase space volume depending on the Lagrange multiplier β , we have an elementary cell which depends on the Lagrange multiplier β (it is a macrocell). We also have the number of cells depending only on the number of particles N (with these positions we may satisfy the requirements to conserve the number of accessible microstates both in extensive and in nonextensive phase volumes Ω_0 and Ω and to preserve the correct form of the equation of state).

3. Application to Classical Ideal Gas: Entropy, Chemical Potential, Free Energy

Classical ideal gas model based on nonextensive thermostatics relations has been the subject of several studies since the first applications of NETS [24, 25]. Classical ideal gas is described by an unperturbed state of a system with long-range interaction and the model can be solved analytically [17]. In the past the equation of state has been derived within several schemes along the steps of evolution of NETS: non-normalized [24, 25], normalized [17], OLM (optimal Lagrange multiplier) [18], incomplete statistics [19, 26, 27], among others.

In this Section we show synthetically that the formally correct equation of state (2.23) obtained by means of the exact expression of the distribution (2.10), can be deduced also in the small deviations case, by taking into account the distribution (2.9) if the macrocells of Eq. (2.25) and of Eq. (2.28) are taken as elementary cells.

The equation of state specific for classical ideal gas remains form invariant under nonextensive generalization of thermodynamics. That is, it is valid for all $q: PV = N / \beta^*$. This means that the equation of state of a NETS classical ideal gas is formally equal to that of extensive statistical mechanics: $PV = N / \beta$.

The Lagrange multiplier β^* previously introduced, associated with the constraint in NETS, is defined by

$$\beta^* = \frac{1}{k_T T_{phys}}, \quad (3.1)$$

k_T is a constant depending on q which becomes the Boltzmann constant k for $q \rightarrow 1$ [18, 28] and T_{phys} , the physical temperature, is

$$T_{phys} = \frac{C_q}{k_T \beta} = \frac{Z_q(\beta)^{1-q}}{k_T \beta} = \left(1 + \frac{1-q}{k_T} S_q^T \right) \frac{1}{k_T \beta}, \quad (3.2)$$

(S_q^T is the Tsallis entropy defined below in Eq.(3.10); in the first treatment of classical ideal gas based on OLM approach [28] the dependence on q was attributed only to k_T and not to T_{phys} or β^*). The partition function $Z_q(\beta)$ is defined by

$$Z_q(\beta) = \frac{V^N}{N!(\Delta\Omega_0)^N} \int \prod_i d^3 p_i n_T, \tag{3.3}$$

where n_T is the square bracket factor of Tsallis distribution [Eq.(2.10)]. Two other quantities that are useful for NETS classical ideal gas calculations are: the coefficient

$$C_q = \frac{V^N}{N!(\Delta\Omega_0)^N} \int \prod_i d^3 p_i \frac{n_T^q}{Z_q(\beta)^q} = Z_q(\beta)^{1-q}, \tag{3.4}$$

and the internal energy

$$U_q = \frac{1}{C_q} \frac{V^N}{N!(\Delta\Omega_0)^N} \int \prod_i d^3 p_i \sum_j \frac{p_j^2}{2m} \frac{n_T^q}{Z_q(\beta)^q}, \tag{3.5}$$

From the explicit expression of Z_q , C_q and U_q (we do not report it here and we send the reader to ref.s [17, 18]), we may verify that the above three functions Z_q , C_q and U_q depend (when $q \neq 1$) on the elementary $\Delta\Omega_0$ as

$$\begin{aligned} Z_q(\beta) &\approx (\Delta\Omega_0)^{-N/(1-Q)}, \\ C_q &\approx (\Delta\Omega_0)^{-N(1-q)/(1-Q)}, \\ U_q &\approx (\Delta\Omega_0)^{-N(1-q)/(1-Q)}, \end{aligned} \tag{3.6}$$

where $Q = 3N(1 - q)/2$.

As well known, when $q \rightarrow 1$ we have that $Z_1 \approx (\Delta\Omega_0)^{-N}$ and C_1 and U_1 do not depend on $\Delta\Omega_0$. The above functions enter into the calculation of the equation of state, which can be derived by means of the usual thermodynamic relations. As we have already discussed in the previous Section, by considering a nonextensive classical ideal gas with distribution function n_i of Eq. (2.9) (small deviations from MB distribution), we have calculated that the equation of state is given by $P V = N k T (1 - 5 \delta + 46 \delta^2)$ i.e., in the limit of small deviations we must have $\beta^* = \beta/C_\delta$ as it can be easily verified.

In fact, within the treatment illustrated in the previous Section, we obtain that in the limit of small deviations and for $3N\delta > 1$ the expression of C_q reduces to C_δ if the elementary cell (macrocell) $\Delta\Omega_0$ of Eq. (2.25) is assumed.

With the expression of $\Delta\Omega$ given by (2.28) in place of $\Delta\Omega_0$ given by (2.25) we obtain that Z_q , C_q and U_q do not explicitly depend on the elementary cell. Z_q and C_q do not depend on β either:

$$Z_q = \frac{\Gamma\left(\frac{2-q}{1-q}\right)}{\Gamma\left(\frac{2-q}{1-q} + \frac{3}{2}N\right)} \frac{N^N}{N!} \left(\frac{1}{1-q}\right)^{3N/2} \left[1 + (1-q)\frac{3}{2}N\right]^{\frac{1}{1-q} + \frac{3}{2}N}, \tag{3.7}$$

and C_q and U_q can be calculated from the relations

$$C_q = Z_q^{1-q}, \quad U_q = \frac{3}{2}N \frac{C_q}{\beta}, \tag{3.8}$$

(the functions $\Gamma(x)$ can be calculated by means of the relation $\Gamma(x) = \sqrt{2\pi} x^{x-1/2} e^{-x}$).

Let us note from Eq. (2.1) that space phase volumes Ω_0 and Ω depend on the elementary cells $\Delta\Omega_0$ and $\Delta\Omega$, respectively. If $\Delta\Omega_0$ is a constant, like h^3 , Ω_0 does not depend on β , but only on N and Ω depends on N and q . Instead, if $\Delta\Omega_0$ has the expression of Eq. (2.25) and $\Delta\Omega$ is given by Eq. (2.28), then Ω_0 is also a function of β and Ω is also a function of β and q .

Let us now derive one of the thermodynamics quantities depending on $\Delta\Omega$, the entropy.

The Boltzmann entropy is defined by

$$S_B = k \ln W_0 = \frac{5}{2} Nk + const. = \frac{5}{2} Nk + Nk \ln \left[\frac{V \left(\frac{2\pi m}{\beta} \right)^{3/2}}{N \Delta\Omega_0} \right], \tag{3.9}$$

where $V(2\pi m/\beta)^{3/2}/\Delta\Omega_0$, is the single particle number of cells.

Taking the elementary cell $\Delta\Omega_0$ given by Eq. (2.25), we obtain $S^B = 5N k/2$ because the single particle number of cells equals N and the value of the constant is zero.

The nonextensive entropy is [4]

$$\begin{aligned} S_q^T &= \frac{k}{1-q} (W^{1-q} - 1) = \frac{k}{1-q} (W_0^{1-q} - 1) \\ &= \frac{k}{1-q} \left\{ \exp \left[\frac{S_B}{k} (1-q) \right] - 1 \right\}, \end{aligned} \tag{3.10}$$

where the condition $W = W_0$ has been used and therefore

$$S_q^T = \frac{5}{2} Nk + (1-q) \frac{25}{8} N^2 k = S_B \left(1 + \frac{5}{2} \delta N \right). \tag{3.11}$$

This relation shows that S_q^T tends to change as N^2 with large N . The chemical potential μ of a classical ideal gas is an intensive quantity, defined by

$$\mu = kT \ln \left[\frac{N}{V} \frac{\Delta\Omega_0}{(2\pi m kT)^{3/2}} \right], \tag{3.12}$$

where $\Delta\Omega_0$ is the elementary cell taken usually equal to h^3 . The quantity μ can be negative or positive and is equal to zero only at the particular value of temperature

$$kT = \left(\frac{N}{V} \right)^{2/3} \frac{h^2}{2\pi m}. \tag{3.13}$$

Considering an ideal classical gas, if we increase the number N of one unity adding, at constant energy and volume, one particle with kinetic energy zero and neglecting all interactions, the number of accessible microstates increases and entropy increases too. Considering the relation

$$\Delta U = T\Delta S - P\Delta V + \mu\Delta N, \tag{3.14}$$

we obtain that μ must be negative. On the contrary, if repulsive interactions are active, the incoming particle increases both the energy of the system and the entropy; the system must spend some energy to return to the initial energy value. Then S_B decreases and sometimes decreases more than the gained quantity because of one more particle in the system. In this case μ is positive.

Let us now take for $\Delta\Omega_0$ the definition of Eq. (2.25). We find that for an extensive ideal classical gas we have $\mu = 0$. This result can be explained because adding one particle at constant energy and

volume the elementary cells decrease their single volumes and the total work done by the system to diminish the spatial volume of $N + 1$ cells is $k T$. Therefore, from Eq.(3.14) we have

$$\mu = \frac{3}{2}kT - \frac{5}{2}kT + kT = 0. \tag{3.15}$$

When the ideal classical gas is nonextensive, using (3.11) the expression of μ is

$$\mu_\delta = -\frac{45}{4}\delta kT - \frac{25}{2}\delta NkT + 46\delta^2 kT, \tag{3.16}$$

which gives $\mu = 0$ when $q \rightarrow 1$ ($\delta = 0$) and is slightly positive or negative depending on the sign of δ . In this case the quantity μ is composed by intensive and extensive terms. Its behaviour versus kT depends on δ and on δN which can be finite or can approach zero or infinity depending on δ and N , separately. To complete our study let us discuss the free energy F . For an extensive ideal classical gas with elementary cell $\Delta\Omega_0$ given by Eq. (2.25) at constant energy and total volume, the function F and its variation due to the addition of one particle to the system are given by the following relations:

$$F = U - T S_B = -N k T, \tag{3.17}$$

$$\Delta F = -k T. \tag{3.18}$$

being $\mu = 0$ and considering the work spent by the system to change the spatial volume of elementary cells.

The variation of free energy of a nonextensive ideal classical gas due to the addition of one particle to the system is, using (3.16)

$$\Delta F_q = -P\Delta V + \mu_\delta = -kTC_\delta + \mu_\delta = -kT\left(1 + \frac{25}{4}\delta + \frac{25}{2}\delta N\right). \tag{3.19}$$

This expression differs from that of the non normalized treatment of Ref. [25]. The NETS free energy (as also defined in Abe et al. [18] and with S_q^T of Eq.(3.10) is

$$F_q = U_q - \frac{S_q^T}{k_T\beta} = -NkT\left(1 + \frac{25}{4}\delta N\right), \tag{3.20}$$

and ΔF_q equals the same quantity calculated above [Eq. (3.19)]. A new definition of free energy introduced by Abe et al. [18] which is

$$F_q = U_q - T \frac{k}{2\delta} \ln C_q = U_q - T \frac{k}{2\delta} \ln\left(1 + \frac{1-q}{k_T} S_q\right), \tag{3.21}$$

gives, by using the elementary cell we have proposed, the same result obtained in Eq. (3.20) and then ΔF_q of Eq. (3.19).

4. Interpretation of the Parameter q

Let us consider again the square fractional deviation from a MB distribution

$$\sum_i \frac{(\partial n_i)^2}{n_{i_0}} = \sum_i \frac{n_i^2}{n_{i_0}} - N = \left(18\delta - \frac{3799}{32}\delta^2\right)N, \tag{4.1}$$

We have already discussed that appreciable fractional deviations are, in general, very small. Nevertheless, few islands of phase space can give a non negligible contribution to deviation of quantities calculated within the standard space, like, for instance, rates of nuclear reactions or atomic processes or rates of chemical reactions. We define, as usual, the radial correlation function

$$g(r) = \frac{V}{N} \sum_{i \neq j} \delta(\bar{r} + \bar{r}_i - \bar{r}_j), \quad (4.2)$$

($g(r) = 1$: perfect gas).

By using the relation

$$\sum_i \frac{(\partial n_i)^2}{n_i} = 1 + \frac{N}{V} \int [g(r) - 1] dr, \quad (4.3)$$

from Eq. (4.1) we can write the following relation:

$$18 \frac{1-q}{2} - \frac{3799}{32} \frac{(1-q)^2}{4} = \frac{1}{N} + \frac{1}{V} \int [g(r) - 1] dr. \quad (4.4)$$

Disregarding, for simplicity, the term in $(1-q)^2$ we have

$$q = 1 - \frac{1}{9} \left\{ \frac{1}{N} + \frac{1}{V} \int [g(r) - 1] dr \right\}. \quad (4.5)$$

Therefore, $q \rightarrow 1$ if both the conditions $g(r) \rightarrow 1$ and $N \rightarrow \infty$ are fulfilled. Otherwise, if $N \rightarrow \infty$ but the system is not a perfect gas [$g(r) \neq 1$]:

$$q = 1 - \frac{1}{9} \frac{1}{V} \int [g(r) - 1] dr, \quad (4.6)$$

and if the system is a perfect gas ($g = 1$) but the number of particles is small and finite:

$$q = 1 - \frac{1}{9N}. \quad (4.7)$$

Finally, in the limit of a gas/fluid of N particles, we have found a physical interpretation of the nonextensive parameter q in terms of the particle correlation function among others (see Wilk et al [6], Beck [7], Beck and Cohen [8] and Tsallis [29]). It can be considered valid at least for values of q not too different from unity, (small deviations from MB distribution).

5. Conclusions

We have calculated the phase space volume Ω and the corresponding elementary cell $\Delta\Omega$, occupied by N classical, identical particles composing a weakly nonextensive system, at equilibrium (or in a steady state, or long-term stationary state of a nonequilibrium system). Both quantities must differ from their extensive MB values Ω_0 and $\Delta\Omega_0$ because we require that the number W_0 of available microstates in the MB extensive phase space Ω_0 equals the number W in the deformed (nonextensive) space: $W_0 = W$. This condition imposes particular analytical expressions of $\Delta\Omega_0$ and $\Delta\Omega$. The number of elementary cells results equal to the number of particles N .

The two elementary cells result to be macrocells if compared to the usually taken elementary cell volume, equal to the third power of the Planck constant, with consequences on the expression of

thermodynamic quantities depending on elementary cell, like, for instance, the partition function, constant of entropy, chemical potential and free energy.

We have applied results on elementary cell to nonextensive classical gas, recovering known results (equation of state) in NETS literature where $\Delta\Omega$ is usually taken equal to h^3 or left undetermined.

We have derived expressions of entropy, chemical potential and free energy and discussed more deeply the case of chemical potential. Applications to particular systems and physical cases like nuclear fusion reactions in plasmas and chemical reactions will be reported elsewhere. Through expressions of Ω and $\Delta\Omega$ we have calculated fractional deviation from Maxwell-Boltzmann distribution. A physical meaning of the nonextensive Tsallis parameter q in terms of the correlation function has been derived.

Acknowledgments

We wish to thank Dr. A.M. Scarfone for critical reading of the manuscript and comments.

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