CBPF-NF-060/95

Grand-Canonical Ensemble Within Tsallis Thermostatistics

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Abstract

Within Tsallis generalized thermostatistics, the grand canonical ensemble is derived for quantum systems. The generalized partition function is also obtained. In addition, the Fermi-Dirac, Bose-Einstein and Maxwell-Boltzmann statistics are defined and the distribution function is generalized as well.

Key-words: Generalized Statistics; Non-extensive Systems; Ideal Gas.

PACS: 05.30-d; 02.50+s; 05.70Ce; 05.90+m

1 Introduction

Non-extensivity (or non-additivity) is an important concept in some areas of physics, by way of reference to some interesting generalizations of traditional concepts. A generalization of the Boltzmann-Gibbs statistics has been recently proposed by Tsallis [1, 2, 3] for non-extensive systems. This generalization relies on a new form for the entropy, namely

$$S_q \equiv -k\frac{1 - Tr(\rho^q)}{1-q},$$

where $q \in \Re$; k is a positive constant. Its standard form introduced by Boltzmann and Gibbs (which yields the correct results for the thermodynamic properties of standard systems) is recovered in the limit $q \to 1$.

Various properties of the usual entropy have been proved to hold for the generalized one [4]; its connection with thermodynamics is now established and suitably generalizes the standard additivity (it is non-extensive if $q \neq 1$) as well as the Shannon theorem [5]. In general, the micro-canonical and canonical formulations have been quite well studied up to now and this formalism has received important applications.

Some aspects of the generalized statistical mechanics in relation to the N-body classical [6, 7] and quantum [8] problems were discussed, in order to treat more general situations than the collisionless one. Now, there exists an attempt to generalize the quantum (Fermi-Dirac and Bose-Einstein) statistics [9], but it was not taken into account the difficulty associated with the concomitant partition function owing to the factorization process shown in [6]. Consequently, the quantum ideal gas has not yet been adequately discussed within generalized statistics.

In the present paper, the formalism in the grand-canonical ensemble is generalized. In Section 2, the generalized grand partition function is obtained; Hilhorst transformations for the partition function and the q-expectation values of the energy and particle number are written. In Section 3, the Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics are defined; the distribution function is generalized in the Hilhorst manner.

2 Open Systems

An open system can exchange heat and matter with its surroundings; therefore, the energy and the particle number will fluctuate. However, for systems in equilibrium we can require that both the average energy and the average particle number be fixed. To find the probability distribution, we need to get an extremum of the entropy which satisfies the above mentioned conditions. We proceed by the method of Lagrange multipliers with three constraints.

2.1 Generalized Grand-Partition Function

We can require that the generalized density operator be normalized over some set of basis states. Thus, the normalization condition takes the form

$$Tr\rho = 1 \quad , \tag{1}$$

the generalized average energy is defined

$$Tr(\rho^q \mathcal{H}) = U_q \ ; \tag{2}$$

it is also called *q-expectation value* [3] of the energy and $\mathcal{H}$ refers to the Hamiltonian of the system. The generalized average particle number is defined

$$Tr(\rho^q \mathcal{N}) = N_q \ . \tag{3}$$

or *q-expectation value* of $\mathcal{N}$ (particle number operator).

To obtain the equilibrium generalized probability distribution, we must find an extremum of the Tsallis entropy subject to the above constraints. The obtained density operator for the grand-canonical ensemble is the following

$$\rho = [1 - \beta(1-q)(\mathcal{H} - \mu\mathcal{N})]^{\frac{1}{1-q}} / \Xi_q(\beta, \mu), \tag{4}$$

where $\beta = 1/kT$. The generalized grand partition function is obtained from Eq.(4) with the aid of Eq.(1)

$$\Xi_q(\beta, \mu) = Tr\,[1 - \beta(1-q)(\mathcal{H} - \mu\mathcal{N})]^{\frac{1}{1-q}} . \tag{5}$$

On the other hand, we can also obtain the fundamental equation for open systems, this takes the following form

$$\Omega_q = -kT \frac{\Xi_q^{1-q} - 1}{1-q}; \tag{6}$$

and it is similar to the fundamental equation for closed systems (canonical ensemble [5]).

2.2 Hilhorst Integral Transformations

The so called Hilhorst integral transformations [2] are important because they connect a thermodynamic or statistical generalized quantity to its respective standard quantity. Therefore, an extension for $q < 1$ of the Hilhorst integral in the Prato style [7] to the grand-canonical ensemble is derived. We obtain

$$\Xi_q(\beta, \mu) = \Gamma(\frac{2-q}{1-q}) \frac{i}{2\pi} \oint_C dz(-z)^{\frac{-1}{1-q}-1} e^{-z} \Xi_1(-\beta(1-q)z, \mu), \tag{7}$$

for $q < 1$. The contour C in the complex plane is depicted in Figure 1. By taking $F(z, \mu) = e^{-z}\Xi_1(-\beta(1-q)z, \mu)$ and $\alpha = 1/(1-q)$; the integral in Eq.(7) can be written as

$$\oint_C dz(-z)^{-\alpha-1} F(z, \mu) = \left(\int_{ab} + \int_{bcd} + \int_{de} \right) dz(-z)^{-\alpha-1} F(z, \mu), \tag{8}$$

where ab, bcd and de are lines of C shown in Figure 1. If we use $z = \xi$ for the integral along the line ab, $z = \epsilon e^{i\theta}$ along the line bcd and $z = \xi e^{2i\pi}$ along the line de, we have

$$\oint_C dz(-z)^{-\alpha-1} F(z, \mu) = \quad -e^{i\alpha\pi} \int_\infty^\epsilon d\xi \xi^{-\alpha-1} e^{-\xi} \Xi_1(-\beta(1-q)\xi, \mu) \tag{9}$$

$$-\epsilon^{-\alpha}e^{i\alpha}\int_0^{2\pi} d(e^{i\theta})(e^{i\theta})^{-\alpha-1}e^{-\epsilon e^{i\theta}}\Xi_1(-\beta(1-q)\epsilon e^{i\theta},\mu)$$
$$-e^{-i\alpha\pi}\int_\epsilon^\infty d\xi\xi^{-\alpha-1}e^{-\xi}\Xi_1(-\beta(1-q)\xi,\mu).$$

Now, putting $q>1$ and $\epsilon\to 0$ we can see that the second integral vanishes. Thus,

$$\oint_C dz(-z)^{-\alpha-1}F(z,\mu) = -2i\sin(\frac{\pi}{q-1})\int_0^\infty d\xi\xi^{\frac{1}{q-1}-1}e^{-\xi}\Xi_1(\beta(q-1)\xi,\mu). \tag{10}$$

On the other hand, we have the following property of the Γ function

$$\Gamma(p)\Gamma(1-p) = \frac{\pi}{\sin\pi p}. \tag{11}$$

Using the Eqs.(10) and (11) into Eq.(7), may be written as

$$\Xi_q(\beta,\mu) = \frac{1}{\Gamma(\frac{1}{q-1})}\int_0^\infty d\xi\xi^{\frac{1}{q-1}-1}e^{-\xi}\Xi_1(\beta(q-1)\xi,\mu), \tag{12}$$

the Hilhorst transformation for $q>1$.

Now, we write similar transformations for the q-expectation value of the energy. It is obtained

$$U_q = \frac{\Gamma(\frac{1}{1-q})}{[\Xi_q(\beta)]^q}\frac{i}{2\pi}\oint_C dz(-z)^{\frac{-1}{1-q}}e^{-z}\Xi_1(-\beta(1-q)z,\mu)U_1(-\beta(1-q)z) \tag{13}$$

for $q<1$; and

$$U_q = \sum_l \frac{1}{[\Xi_q(\beta)]^q\Gamma(\frac{q}{q-1})}\int_0^\infty d\xi\xi^{\frac{1}{q-1}}e^{-\xi}\Xi_1(\beta(q-1)\xi,\mu)U_1(\beta(q-1)\xi) \tag{14}$$

for $q>1$ (for the canonical ensemble it is shown in [10]).

Similar expressions are obtained for the q-expectation value of the particle number

$$N_q = \frac{\Gamma(\frac{1}{1-q})}{[\Xi_q(\beta)]^q}\frac{i}{2\pi}\oint_C dz(-z)^{\frac{-1}{1-q}}e^{-z}\Xi_1(-\beta(1-q)z,\mu)N_1(-\beta(1-q)z) \tag{15}$$

for $q<1$; and

$$N_q = \frac{1}{[\Xi_q(\beta)]^q\Gamma(\frac{q}{q-1})}\int_0^\infty d\xi\xi^{\frac{1}{q-1}}e^{-\xi}\Xi_1(\beta(q-1)\xi,\mu)N_1(\beta(q-1)\xi) \tag{16}$$

for $q>1$.

3 Quantum Ideal Gases

We choose as basis states the number representation where $\mathcal{H}$ and $\mathcal{N}$ are diagonal whose eigenvalues are $E_L^{(N)}$ and N respectively. The number of particles $N=0,1,2...$, and $E_L^{(N)}$ represents the N-particle energy spectrum (characterized by the quantum number or set of quantum numbers L). Thus, we can obtain the equilibrium distribution for the grand-canonical ensemble from Eq. (4), this is

$$p_L^{(N)} = \left[1 - \beta(1-q)(E_L^{(N)} - \mu N)\right]^{\frac{1}{1-q}} / \Xi_q(\beta, \mu). \tag{17}$$

It is convenient to remark that in general

$$p_N \equiv \sum_L p_L^{(N)} \neq \left[\sum_L \left[p_L^{(N)}\right]^q\right]^{1/q} \equiv p^{(N)} \tag{18}$$

where p_N is the probability of having N particles (no matter the energy value) and $p^{(N)}$ is the quantity which enables us re-writting Eq.(3) as $\sum_{N=0}^{\infty} N \left[p^{(N)}\right]^q = N_q$; unless $q = 1$, p_N generically differs from $p^{(N)}$ (for instance, $\sum_{N=o}^{\infty} p_N = 1$ always, whereas in general $\sum_{N=0}^{\infty} p^{(N)} \neq 1$).

In this representation Eq.(5) is

$$\Xi_q(\beta, \mu) = \sum_{N=0}^{\infty} \sum_L \left[1 - \beta(1-q)(E_L^{(N)} - \mu N)\right]^{\frac{1}{1-q}}. \tag{19}$$

3.1 Quantum Statistics

The statistics of N-body quantum systems plays a crucial role in determining the thermodynamic behavior at very low temperature. It is known however that, in the standard framework, there is no difference between Bose-Einstein and Fermi-Dirac statistics at high temperature. Maxwell-Boltzmann statistics is the name given to the statistics which describes the behavior of the systems at high temperature.

When evaluating the trace in Eq.(5) or the set of quantum numbers L in Eq.(19) we must be careful to count each possible state of the system only once. If the quantum state of the system is specified by the one-particle states. The total energy is given by

$$E_L^{(N)} = \epsilon_{l_1} + \epsilon_{l_2} + \ldots + \epsilon_{l_N},$$

where ϵ_{l_i} is the energy of the single particle i.

Then, the generalized grand partition function for the Maxwell-Boltzmann statistics can be written as

$$\Xi_q^{M-B} = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{l_1} \sum_{l_2} \ldots \sum_{l_N} [1 - \beta(1-q)(\epsilon_{l_1} + \epsilon_{l_2} + \ldots + \epsilon_{l_N} - N\mu)]^{\frac{1}{1-q}}, \tag{20}$$

where we have inserted the factor $1/N!$ in the same way as in the $q = 1$ statistics, because it gives us the proper form of the grand partition function for indistinguishable particles at high temperature.

We consider particles with periodic boundary conditions as a simple application of Eq.(7) and Eq. (20). If the volume is large enough, the particle energies will be closely spaced and we can replace the sum over l by an integral over a continuous variable k. Thus,

$$\sum_{l=-\infty}^{\infty} e^{-\beta\epsilon_l} \to \left(\frac{\ell}{2\pi}\right)^D \frac{2\pi^{D/2}}{\Gamma(D/2)} \int_0^\infty dk k^{D-1} e^{-\beta\hbar^2 k^2/2m}, \tag{21}$$

where D is the dimension. Hence, when $q = 1$, Eq.(20) becomes

$$\Xi_1^{M-B} = \sum_{N=0}^{\infty} \frac{e^{N\beta\mu}}{N!} \left[\sum_l e^{-\beta\epsilon_l}\right]^N = \sum_{N=0}^{\infty} \frac{1}{N!} e^{N\beta\mu} \left(\frac{m\ell^2}{2\pi\hbar^2\beta}\right)^{ND/2}, \tag{22}$$

Replacing Eq.(22) into Eq.(7), we obtain:

$$\Xi_q^{M-B} = \sum_{N=0}^{\infty} \frac{\Gamma(\frac{2-q}{1-q})[1+\beta(1-q)\mu N]^{\frac{1}{1-q}+\frac{ND}{2}}}{N!(1-q)^{DN/2}\Gamma(\frac{2-q}{1-q}+\frac{ND}{2})} \left(\frac{m\ell^2}{2\pi\hbar^2\beta}\right)^{ND/2}, \tag{23}$$

for $q < 1$, this is the high-temperature approach. Eq.(22) is recovered from Eq.(23) in the limit $q \to 1$.

The generalized grand partition function in Fermi-Dirac statistics, according to Pauli exclusion principle, is given by

$$\Xi_q^{F-D} = \sum_{N=0}^{\infty} \sum_{l_1}^{\infty} \sum_{l_2=l_1+1}^{\infty} \cdots \sum_{l_N=l_{N-1}+1}^{\infty} [1-\beta(1-q)(\epsilon_{l_1}+\epsilon_{l_2}+\ldots\epsilon_{l_N}-N\mu)]^{\frac{1}{1-q}}. \tag{24}$$

Each different set of occupation numbers corresponds to one possible state.

The generalized grand partition function in Bose-Einstein statistics is given by

$$\Xi_q^{B-E} = \sum_{N=0}^{\infty} \sum_{l_1}^{\infty} \sum_{l_2=l_1}^{\infty} \ldots \sum_{l_N=l_{N-1}}^{\infty} [1-\beta(1-q)(\epsilon_{l_1}+\epsilon_{l_2}+\ldots+\epsilon_{l_N}-N\mu)]^{\frac{1}{1-q}}. \tag{25}$$

Here, there is no restriction on the number of particles that can occupy a given momentum state.

Low-temperature approach for fermions with periodic boundary conditions and chemical potential computations as a function of the temperature for the particles in a box problem are shown in [8].

3.2 Generalized Distribution Function

Finally, let us also write the generalized distribution function in the Hilhorst manner. We remark that a multiple sum appears by evaluating the trace in Eqs.(1)-(3) and (5). That multiple sum can be transformed into a unique sum over some set of basis states of non-interacting particles, by standard methods.

Now, let us remember that

$$N_1 = \sum_l n_{1l}, \tag{26}$$

where n_{1l} is known as the distribution function and it is very well defined in the Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. By replacing Eq.(26) into Eq.(15) and Eq.(16), we obtain the generalized distribution functions. We define

$$n_{ql} = \frac{\Gamma(\frac{1}{1-q})}{[\Xi_q(\beta)]^q} \frac{i}{2\pi} \oint_C d\xi (-\xi)^{\frac{-1}{1-q}} e^{-\xi} \Xi_1(-\beta(1-q)\xi) n_{1l}(-\beta(1-q)\xi) \tag{27}$$

for $q < 1$; and

$$n_{ql} = \frac{1}{[\Xi_q(\beta)]^q \, \Gamma(\frac{q}{q-1})} \int_0^\infty d\xi \xi^{\frac{1}{q-1}} e^{-\xi} \Xi_1(\beta(q-1)\xi) n_{1l}(\beta(q-1)\xi) \tag{28}$$

for $q > 1$. Therefore, we have defined the generalized distribution functions in connection with the standard distribution and partition functions through Eq.(27) and Eq.(28). In addition, we have

$$N_q = \sum_l n_{ql} \tag{29}$$

which is the generalization of the Eq.(26).

Conclusions

Clearly, the statistical and thermodynamic quantities recover their standard forms in the $q \to 1$ limit.

The connection between generalized statistical mechanics in the grand canonical ensemble and thermodynamics is well established through the relation given by Eq.(6).

Following along the lines of the Hilhorst integral transformations for the grand partition function Ξ_q, we have obtained the analogous expressions for the appropriate averages of the particle number and the energy in the grand-canonical ensemble. In the same style, the generalized distribution functions are defined as well.

Acknowledgments

The author is very indebted to Constantino Tsallis for valuable discussions and to Celia Anteneodo for their helpful comments on the draft version of this paper. The author has also benefitted from financial support from the CLAF/CNPq.

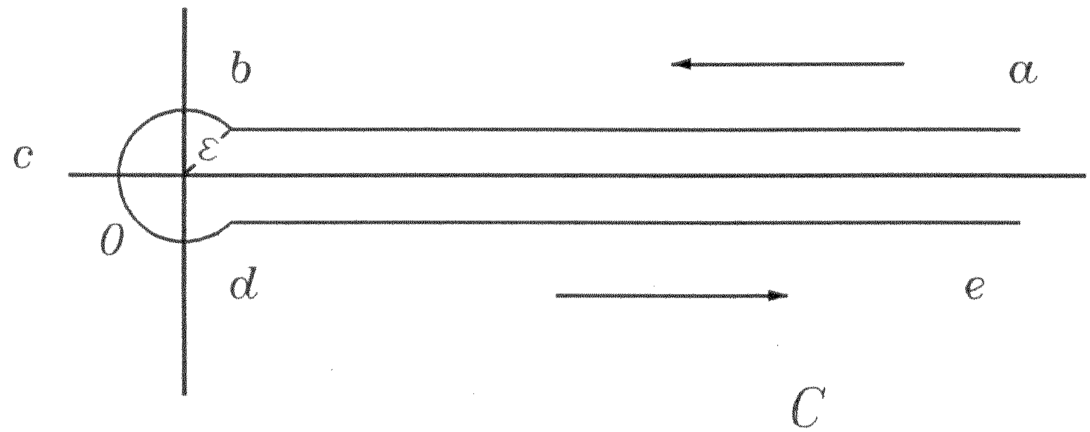

Figure 1

Contour C in the complex plane.

References

[1] C. Tsallis, J. Stat. Phys. **52** (1988) 479 .

[2] C. Tsallis, in "New Trends in Magnetism, Magnetic Materials and their Applications", ed. J. L. Morán-Lopez and J. M. Sánchez (Plenum Press, New York, 1994) 451.

[3] C. Tsallis, Chaos, Solitons and Fractals **6** (1995) 539.

[4] A. M. Mariz, Phys. Lett. **A 165** (1992) 409; J. D. Ramshaw, Phys. Lett. **A 175** (1993) 169; J. D. Ramshaw, Phys. Lett. **A 175** (1993) 171.

[5] E. M. F. Curado and C. Tsallis, J. Phys. A: Math. Gen **24** (1991) L69; Corrigenda: J. Phys. A**24** (1991) 3187 and **25** (1992) 1019.

[6] A.R.Plastino, A.Plastino and C. Tsallis, J. Phys. A: Math. Gen **27** (1994) 1.

[7] D. Prato, Phys. Lett. **A 203** (1994) 165.

[8] S. Curilef, *"Generalized Statistical Mechanics for the N-body Quantum Problem – Ideal Gases"* (1995) preprint.

[9] F. Büyükkiliç and D. Demirhan, Phys. Lett. **A 181** (1993) 24; F. Büyükkiliç, D. Demirhan and A. Güleç, Phys. Lett. **A 197** (1995) 209.

[10] S. Curilef and C. Tsallis, Physica **A 215** (1995) 542.