Geometric aspects in Equilibrium Thermodynamics

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We discuss different aspects of the present status of the Statistical Physics focusing the attention on the non-extensive systems, and in particular, on the so called small systems. Multimicrocanonical Distribution and some of its geometric aspects are presented. The same could be a very attractive way to generalize the Thermodynamics. It is suggested that if the Multimicrocanonical Distribution could be equivalent in the Thermodynamic Limit with some generalized Canonical Distribution, then it is possible to estimate the entropic index of the non-extensivethermodynamics of Tsallis without any additional postulates.

I. INTRODUCTION

Traditionally, the Statistical Physics and the standard Thermodynamics have been formulated to be applied to the study of extensive systems, in which the consideration of the additivity and homogeneity properties, as well as the realization of the Thermodynamical Limit are indispensable ingredients for their performance. The study of these systems is based on the consideration of the extensive Shannon-Boltzmann-Gibbs entropy [1]:

\[ S_E = - \sum_k p_k \ln p_k \] (1)

which satisfied the additivity and concavity conditions. This definition is the base of the well known H theorem of Boltzmann, which is connected with the Second Law of the Thermodynamic [2], the law of the growth of the entropy. This definition leads, during the thermodynamical equilibrium, to the description of such systems by means of Boltzmann-Gibbs Distributions[1]:

\[ \omega_{B-G}(X; I, N, a) = \frac{1}{Z(\beta, N, a)} \exp \left[ -\beta \cdot I_N(X; a) \right] \] (2)

In fact, by means of this formalism, it is possible to obtain sound results when it is applied to physical systems in which the above mentioned conditions are valid i.e., to systems satisfying the homogeneity and additivity conditions. However, these conditions can not be inferred from general principles. Nowadays, these properties can be considered as reasonable approximations for systems containing many particles interacting by means of short range forces[3 – 5], being these systems homogeneous from the macroscopic point of view, so that they are not suffering a phase transition of first order [6, 7]. Out of this context, the applicability of this theory arouse to be doubtful.

In the last years considerable efforts have been devoted to the study of non-extensive systems. The available and increasingly experimental evidences on anomalies presented in the dynamical and macroscopical behavior in plasma and turbulent fluids [8 – 11], astrophysical systems [12 – 17], nuclear [18, 19] and atomic clusters [20], granular matter [21], glasses[22, 23] and complex systems [24], constitute a real motivation for the generalization of the Thermodynamics.

II. RECENT DEVELOPMENTS

A step forward in these studies have been advanced in 1988 with the proposal of Constantino Tsallis [25] (see also [26, 27]). In [25] he considered a generalization of the Boltzmann-Gibbs formalism to take into account the non-extensive characteristics of a system introducing the non-extensive entropy, \( q \)-entropy, \( S_q \):

\[ S_q = \frac{1 - \sum_k p_k^q}{q - 1} \] (3)

In this case, \( q \), the entropic index, is a parameter that describes the non extensive character of the system. It can be demonstrated that when \( q \) approaches to the unit the \( q \)-entropy becomes in the traditional extensive one. In the case of the systems in thermodynamic equilibrium, this definition generalizes the Boltzmann-Gibbs distributions:
\[ \omega_q (X; I, N, a) = \frac{1}{Z_q (\beta, N, a)} [1 - (1 - q) \beta \cdot I_N (X; a)]^{\frac{1}{1-q}} \] (4)

substituting this way the exponential laws for potential laws.

It is important to remark that with this kind of description one can obtain good results when it is applied to a broad variety of non extensive and complex systems. For example, in the case of non lineal systems, this concept has leaded to generalize the Sinai-Komolgorov entropy, allowing the study of chaotic regimes that could not be well described by other formalisms [28]. However, one should mention that the formalism can be classified as a parametrical one, since q can not be estimated a priori for a given system and can not be derived from general principles. In fact, it acts as an adjustment parameter.

In the last years there are important progresses in studying small systems, understanding for such, those systems whose interaction range is long comparable to or longer than the linear dimensions of the system. Under this denomination can be grouped the molecular and atomic clusters and even the astrophysical systems, confined under their own gravity, among others.

For such systems, the postulates of the traditional statistical physics do not take place, because they are not homogeneous, their integrals of movements are non additive, and they can not necessarily be considered as systems of many particles. On the other hand, it is generally accepted, in the framework of the standard theory, that the phase transitions only can take place in systems which reach the thermodynamic limit, composed by a huge number of particles. The study of the properties of the finite nuclear matter has revealed experimental evidences of the occurrence of phase transitions of first order during the nuclear multifragmentation [29], forcing us to change our conceptions in this respect.

It is not difficult to notice of the great proximity that has the no-extensive formulation of the thermodynamic given by Tsallis with their antecedent, the Standard Thermodynamic:

- Both are based on a probabilistic interpretation for the entropy, characteristic that allows a great versatility for the application of this important concept to other fields.

- A common denominator of both theories is the consideration of the thermodynamic limit, the limit of many particles. In this way, the description of the macroscopic state of equilibrium systems is carried out by means of the parameters of the generalized canonical distributions and therefore paying a full attention to the validity of the zero principle of the Thermodynamics.

Here the reason that these theories can not be applicable to those systems composed by few bodies, and in general, to the small systems. If we want to arrive to a more general statistical formulation, it is necessary to abandon definitively the postulates of the traditional theory. In this line, there are important contributions of Prof. Gross at Hahn Meitner Institute of Berlin who developed a formalism for analyzing the nuclear multifragmentation and the statistical mechanics of small systems by means of the Microcanonical Thermostatistics[30, 31].

To reach their objective, the same one returned at the pre-Gibbsians times, reconsidering the entropy concept given by Boltzmann, the celebrated epitaph of his gravestone in Vienna:

\[ S_B (E, N, a) = \ln (W (E, N, a)) \] (5)

where:

\[ W (E, N, a) = \Omega (E, N, a) \delta \epsilon = \int dX \delta [E - H_N (X; a)] \delta \epsilon \] (6)

with the consideration of the ordinary Microcanonical Distribution for the closed systems:

\[ \omega_M (X; E, N, a) = \frac{1}{\Omega (E, N, a)} \delta [E - H_N (X; a)] \] (7)

From this base, the deduction of the Thermodynamic can only be developed starting from the principles of the mechanics, without appealing to other considerations. At this point it is necessary to stress the hierarchy of the microcanonical ensemble regarding the other statistical ensembles as pointed out by Boltzmann[32], Gibbs[7], Einstein[33, 34], Ehrenfests[35] because the Canonical and Grand Canonical ensembles can be derived from the Microcanonical one through of certain particular conditions: the extensity postulates.

The meaning of the Boltzmann entropy is very direct, physically palpable, valid for any system of particles, independently whether it is formed of many particles or not: it is equal to the logarithm of the volume of the hypersurface
of constant energy in the N-body phase space of the system. By this way, the Boltzmann entropy is a bridge, a direct connection between the microscopic characteristics of the system with their macroscopic properties.

Nevertheless the achievements of the formalism, exist reasons to believe that this is not still a completed one:

- It is characteristic for this formulation the relevance of the ergodic chauvinism of the traditional distributions. This is translated as the preference of the energy on all the integral of movement corresponding to the system.
- The consideration of the Boltzmann entropy is limited to the equilibrium and therefore this important concept can not be extended to the kinetics[36].

Many of the systems traditionally described by the Statistical Physics are considered located in certain region of the space due to the action of a external confining field. It is the reason to consider and justify this preference since among the integral of movements (the energy, the impulse and total angular moment), the energy is only one conserved.

However, there is some systems in which the energy is not enough to describe their macroscopic state and it is also necessary the consideration of the total angular moment and other integral of movement in general . This necessity becomes evident when we tried to make the macroscopic description of the nucleus, as well as when we deal with the astrophysical systems[37,38].

These are the antecedents of the which starts the formulation of the Multimicrocanonical Distribution[39,40]. As their precedent, this formulation pretend to be essentially geometric, characteristic that not only could facilitate handling this distribution, but it could have also deeper consequences in the understanding of the Statistical Physics of the systems in equilibrium thermodynamics .

III. GEOMETRICAL ASPECTS OF THE MULTIMICROCANONICAL DISTRIBUTION

Let \((I,N,a)\) represent the macroscopic state of a system, where \(I \equiv \{I^1, I^2 \ldots I^n\}\) are the set of integrals of movement of the distribution, \(N\) the particle number and \(a\) describe an external parameter. Following the general ideas of the Microcanonical Thermostatistic, the probability phase density is given by:

\[
\omega_M (X; I, N, a) = \frac{1}{\Omega (I, N, a)} \delta (I - I_N (X; a)) \tag{8}
\]

generalizing the ordinary microcanonical distribution, where \(\Omega\) is the state density. The choice of equal-probability hypothesis allows to take a totally geometrical version for the statistic mechanics without the introduction of artificial elements in the formulation.

Similarly, we assumed the Boltzmann’s definition of entropy:

\[
S_B (I, N, a) = \ln (\Omega (I, N, a) \delta I) \tag{9}
\]

where \(\delta I\) is a suitable elemental volume. The Boltzmann definition of entropy does not require to satisfy the concavity and extensity conditions that ordinary exhibits the information entropy. How we can see, this definition is essentially geometrical and transparent in its sense.

As we showed in Ref. [40], in this formulation appears the concepts of scalar product and divergency of vectors belonging to a geometrical approach. It motived to develop a geometrical formalism to work with this distribution. The geometrical aspects of the theory are summed up by the following facts:

- Any function of the movement integrals is itself a movement integral. If we have a complete independent set of functions of the movement integral of the distribution, then this set of functions is equivalent to the other set of movement integrals, representing the same macroscopic state of the system. That is why it is more exactly to speak about an abstract Space of movement integrals for the multimicrocanonical distribution, \(\Im N\).
- Every physical quantity or behavior has to be equally reproduced by any representation of the space of macroscopic state, \((\Im N; a)\).

- It is easy to show that the multimicrocanonical distribution is local reparametrization invariant. Let \(\Im I\) and \(\Im \phi \ (I \equiv \{I^1, I^2 \ldots I^n\} , \phi \equiv \{\phi^1 (I), \phi^2 (I) \ldots \phi^n (I)\})\) two representations of \(\Im N\). By the property of the \(\delta\)-function we have:
\[
\delta [\phi (I) - \phi (I_N (X; a))] = \left[ \frac{\partial \phi}{\partial I} \right]^{-1} \delta [I - I_N (X; a)]
\] (10)

hence:

\[
\tilde{\Omega} (\phi, N, a) = \left[ \frac{\partial \phi}{\partial I} \right]^{-1} \Omega (I, N, a)
\] (11)

and therefore:

\[
\omega_M (X; \phi, N, a) = \omega_M (X; I, N, a) \equiv \omega_M (X; \Im^N, a)
\] (12)

- The state density allows to define the invariant measure of the space:

\[
d\mu = \Omega (I, N, a) \, d^n I
\] (13)

although this is the most important measure for the space, this is not the only one, because there are others like them derived from Poincare invariants, when we project the N-body phase-space to the space \(\Im^N\).

- The movement integrals are defined by the commutativity relation with the Hamiltonian of the system. In the case of closed systems, the Hamiltonian is the energy of the system, and this is a conserved quantity. In the multicrocanonical distribution it represents one of the coordinate of the point belonging to \(\Im^N\), in an specific representation. When we change the coordinate system, the energy lose its identity. Since we can not fix the commutativity of the energy with the others integrals, it would be more correct that all movement integrals commute between them in order to preserve these conditions. Thus, we make consistently the local reparametrization invariance with the commutativity relations. As we see, still from the classical point of view, the reparametrization invariance suggests that the set of movement integrals have to be simultaneously measured. In the quantum case, this is an indispensable request for the correct definition of the statistical distribution. This property is landed to the classical distribution by the correspondent principle between the Quantum and the Classic Physic.

This reparametrization freedom is very attractive: we can choose the representation of the macroscopic state space more adequate to describe the statistical system. There are many examples in which an adequate choice of coordinate system helps us to simplify the resolution of a problem.

Let us move now to the Boltzmann definition of entropy. Obviously it has to be an scalar function. Its value can not depends on the coordinate system used to describe the macroscopic state. It is our interest that this function characterizes the macroscopic state of the system, it have to allow us to get information about the ordering of it. In this case, \(\delta I\) can not be arbitrary. It has to be a characteristic of the representation of the space \(\Im^N\).

These facts aim toward the creation of a statistical theory conceived as a local geometric theory. To achieve this it should be endowed to the space \(\Im^N\) of a geometric structure: we have to introduce a theory of tensors and vectors and incorporate the covariant differentiation, local bases, etc. We are interested in describing those properties of system possessing topological and geometrical invariance, since they represent characteristics illustrating the behavior of the system.

**IV. GENERAL PERSPECTIVES.**

By taking into account the previous discussions, the problem is reduced to endow the space of the movement integrals of the system, \(\Im^N\), of a geometric structure. When we speak on a geometric structure, we are referring to consider it as a topological and metric space. This aspect is not new in the statistical physics. An antecedent of this approach is the geometric interpretation make by Weinhold [41] to the Standard Thermodynamic for extensive systems. However, this approach is not valid for a more general case.

A paradigmatic point in this direction is the supposition of the existence of a internal product among vectors in this space, it means, the consideration of a metric tensor \(g_{\mu \nu}\). It constitutes the basis for the definition of invariant quantities and of the covariant differentiation[42].

Having in mind the fundamental character that this concept has for the theory, it is not difficult to admit that a possible and reasonable generalization of the Boltzmann entropy should be:
\[ S_B = \ln \left[ \frac{\Omega (I, N, a)}{\sqrt{|g|}} \right] \] (14)

where \( g = \det (g_{\mu \nu}) \). In this way, the Boltzmann entropy results an scalar function, allowing the characterization of the macroscopic state of the system.

Are very well-known the difficulties presented during the initial development of the statistical mechanics, because it was a theory based in the microscopics laws of the classic physics, a theory on the continuous. These difficulties were overcome only with the arriving of the quantum Physics. It is very well-known too how Boltzmann appeals to the idea of the quantification in order to deal with a well defined definition of entropy, consideration that years later was consider by Planck in the interpretation of the very celebrated formula for the of emission spectrum of the black body\[43\]. This is a very interesting connection between the quantum theory with the statistical mechanics.

The consideration of a geometric structure for the space \( \mathcal{S}_N \) is an alternative for the correct definition of the statistics. The metric tensor should be derived from magnitudes that have their origin in the principles of the mechanics. The same one should be derived starting from certain structural equations whose form we still ignores. However, for the completeness of the theory, these equations should be intimately bond to the quantum properties of the systems.

An essentially important fact for this theory is that the same one presents two general symmetries: it is invariant under the local reparametrizations or diffeomorfism of \( \mathcal{S}_N \), \( \text{Diff}(\mathcal{S}_N) \), and under the transformations of the unitary lineal group, \( \text{SL}(n, \mathbb{R}) \).

It is necessary to recall that the first one constitutes the maximum symmetry that a theory of geometric character can possess, associating it to the multimicrocanonical distribution. On the other hand, the transformations of the unitary lineal group \( \text{SL}(n, \mathbb{R}) \) constitutes the group of more general symmetry that possess the distributions of Boltzmann-Gibbs and of the derived potential distributions of the theory of Tsallis. In this case, these transformations should respect the properties of scaling of the movements integral for these distributions. To be more specific, in the peculiar case of the distributions of Boltzmann-Gibbs these transformations respect the additivity of the integrals of movement. This symmetry group acts on the space vectorial tangent to each point of the space \( \mathcal{S}_N \), i.e., an euclidean space.

In the particular case of the extensive systems, if we considered the thermodynamic limit in the representation of the space \( \mathcal{S}_N \) through the additives integral of movement, the multimicrocanonical distribution degenerates in the Boltzmann-Gibbs distributions. This fact, together with the consideration of the thermodynamic limit lead to a rupture of the symmetry from \( \text{Diff}(\mathcal{S}_N) \) to \( \text{SL}(n, \mathbb{R}) \), from a curved to euclidean space.

If we extrapolate this interpretation to the general case, the Multimicrocanonical Distribution would become what we denominate a Parent Theory for all the Statistical Distributions for the systems in macroscopic equilibrium when the thermodynamic limit is reached. The Boltzmann entropy would allow a probabilistic interpretation to the style of Shannon-Boltzmann-Gibbs entropy and the non extensive entropy of Tsallis. In the last case, it is really interesting point because open the door to a possibility to obtain the entropic index \( q \) without the necessity of appealing to additional postulates.

V. CONCLUSIONS

The geometrical interpretation of the equilibrium thermodynamics is a very interesting way to generalize it. The Boltzmann definition of entropy is the most transparent connection between the Microscopical and Statistical Mechanics, and it is probable the only way to extended the thermodynamics to the few-body systems. If the Multimicrocanonical Distribution could be equivalent in the Thermodynamic Limit with some generalized Canonical Distribution, then it is possible to estimate the entropic index of the non-extensive thermodynamics of Tsallis without any additional postulates.

REFERENCES

[1] R.Balian, From Microphysis to Macrophysics. Methods and applications of Statistical Physics, Volume I, Springer-Verlag, 1991.
[2] Y.Telieski, Física Estadística, Editorial Pueblo y Educación, Instituto Cubano del Libro, 1968.
[3] R.K. Pathria, Statistical Mechanics , Butterworth Heinemann 1996.
[4] H.E. Stanley, Introduction to Phase Transitions and Critical Phenomena, Oxford University Press, New York 1971.
[5] P.T. Landsberg, Thermodynamics and Statistical Mechanics, Dover 1991.
[6] L. Tisza, Annal. Phys. B, 1, (1981); Generalized Thermodynamics, MIT Press, Cambridge, 166, page 123.
[7] J.W. Gibbs, Elementary Principles in Statistical Physics, Volume II of The Collected works of J. Williard Gibbs, Yale University Press, 1902.
[8] B.M. Boghsonian, Phys. Rev. E 53 (1996) 4754.
[9] C. Beck, G.S. Lewis and H.L. Swinney, Phys. Rev. E 63 (2001) 035303(R).
[10] T.H. Solomon, E.R. Weeks and H.L. Swinney, Phys. Rev. Lett. 71 (1993) 3975.
[11] M.F. Shlesinger, G.M. Zaslavsky and U. Frisch Eds., Lévy flights and related topics, Springer-Verlag Berlin (1995).
[12] D. Lynden-Bell, Physica A 263 (1999) 293.
[13] F. Sylos Labini, M. Montuori and L. Pietronero, Phys. Rep. 293 61 (1998) 61.
[14] L. Milanovic, H.A. Posch and W. Thirring, Phys. Rev. E 57 (1998) 2763.
[15] H. Koyama and T. Konishi, Phys. Lett. A 279 (2001) 226.
[16] A. Torcini and M. Antoni, Phys. Rev. E 59 (1999) 2746.
[17] D.H.E. Gross, Microcanonical thermodynamics: Phase transitions in Small systems, 66 Lectures Notes in Physics, World scientific, Singapore (2001) and refs. therein.
[18] M. D’Agostino et al., Phys. Lett. B 473 (2000) 219.
[19] M. Schmidt, R. Kusche, T. Donges and W. Kronmueller, Phys. Rev. Lett. 86 (2001) 1191.
[20] A. Kudrolli and J. Henry, Phys. Rev. E 62 (2000) R1489.
[21] G. Parisi, Physica A 280 (2000) 115.
[22] P.G. Benedetti and F.H. Stillinger, Nature 410 (2001) 259.
[23] G.M. Viswanathan, V. Afanasyev, S.V. Buldyrev, E.J. Murphy and H.E. Stanley, Nature 393 (1996) 413.
[24] C.Tsallis, J. Stat. Phys. 52, 479 (1988).
[25] C.Tsallis, Nonextensive Statistic: Theoretical, Experimental and Computational evidences and connections, Brazilian J. of Phys., Vol. 29, no. 1 (1999).
[26] A set of mini-reviews is available in Nonextensive Statistical Mechanics and Thermodynamics, eds. S.R.A. Salinas and C. Tsallis, Braz. J. Phys. 29 (1999) [http://sbf.if.usp.br/WWWpages/Journals/BJP/Vol29/Num1/index.htm]; C. Tsallis, in Nonextensive Statistical Mechanics and its Applications, eds. S. Abe and Y. Okamoto, Lecture Notes in Physics (Springer-Verlag, Berlin, 2000), in press.
[27] U. Tirnakli, G.F.J. Garin, C. Tsallis, Generalization of the Komolgorov-Sinai entropy: Logistic- and Periodic-like maps at a Chaos Thresholds, [http://arXiv.org/abs/cond-mat/0005210).
[28] L. Moretto et al., Phys. Lett. L76 (1996), 372-5.
[29] D.H.E. Gross, Microcanonical Statistical Mechanics of some non extensive systems, [http://arXiv.org/abs/cond-mat/0004268).
[30] D.H.E. Gross, Microcanonical Thermodynamics and statistical fragmentation of dissipative systems- the topological structure of N-body phase space, Phys. Report, 257:133-221(1995).
[31] L. Boltzmann, Über die Beziehung eines allgemeinen mechanischen Satzes Zum Hauptsatz der Wärmelehre. Sitzungsbericht der akademie der Wissenschaften, Wien, II:67-73, 1877.
[32] A. Einstein, Eine Theorie der Grundlagen der Thermodynamik, Annal. Phys 11:170-187, 1903.
[33] A. Einstein, Zur allgemeinen molekularen. Theorie der Wärme, Annal. Phys 14:354-362, 1904.
[34] P. Ehrenfest and T. Ehrenfest. The conceptual Foundation of the Statistical Approach in Mechanics, Cornell University Press, Ithaca NY, 1959.
[35] This author consider this problem in a recent paper, see in D.H.E. Gross, Second law of Thermodynamics and macroscopic Observables within Boltzmann’s principle, an attempt, [http://arXiv.org/abs/cond-mat/0011130).
[36] O. Fleigang, D.H.E. Gross, The effect of angular conservation on equilibrium properties of selfgraviting systems, [http://arXiv.org/abs/cond-mat/0102062).
[37] V. Laliena, The effect of angular conservation conservation in the phase transition of collapsing systems, Phys. Rev. E 59, 4786 (1999); [http://arXiv.org/abs/cond-mat/9806241).
[38] L. Velazquez, F. Guzman, Thesis of graduation, Instituto Superior de Ciencias y Tecnologías Nucleares, La Habana, 2000.
[39] L. Velazquez, F. Guzman, Some geometrical aspects of microcanonical distribution, [http://arXiv.org/abs/cond-mat/0102459).
[40] F. Weinhold, Metric geometric of Equilibrium Thermodynamics, J. Chem. Phys. 63(1975), 2479-2501.
[41] L. Santalo, Vectores, tensores y sus aplicaciones, Buenos Aires, 1966.
[42] L. Polak, El nacimiento de la Física Cuántica, Las Ideas básicas de la Física, page 335, Ediciones Pueblos Unidos, Montevideo, Uruguay, 1962.