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Thermodynamic geometry for a non-extensive ideal gas

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A generalized entropy arising in the context of superstatistics is applied to an ideal gas. The curvature scalar associated to the thermodynamic space generated by this modified entropy is calculated using two formalisms of the geometric approach to thermodynamics. By means of the curvature/interaction hypothesis of the geometric approach to thermodynamic geometry it is found that as a consequence of considering a generalized statistics, an effective interaction arises but the interaction is not enough to generate a phase transition. This generalized entropy seems to be relevant in confinement or in systems with not so many degrees of freedom, so it could be interesting to use such entropies to characterize the thermodynamics of small systems.

1. Introduction

Because of the existence of anomalous systems which do not seem to obey the rules of common statistics generally associated to non-equilibrium processes, a more general statistics has been proposed [1] based on superstatistics [3,2] which considers large fluctuations of intensive quantities [2]. We review here this formulation in which the intensive fluctuating quantity is the temperature. This fluctuation gives rise to a certain probability distribution characterized by a generalized Boltzmann factor. We can, in principle, associate an entropy for every probability distribution and in this context the Boltzmann–Gibbs entropy corresponds to the usual Boltzmann factor. It is, however, possible to obtain other generalized expressions for entropies associated to different probability distributions [4] depending on one or several parameters [3,5]. In [1,5], it was shown how to generate an entropy depending only on the probability. The particular entropy considered here arises from a generalized gamma distribution depending only on the probability p_l. This entropy has several interesting features and it seems to be relevant for particular thermodynamic systems like confined systems [6] and in this context we find an interesting and necessary application of such generalized entropies. The quantum version of this entropy which is a generalization of the Von Neumann entropy arises by means of a natural generalization of the replica trick [7–9].

In the formalism of the geometric approach to thermodynamics, a geometric structure is given for usual thermodynamic systems by means of Riemannian geometry [10–12,15,13,14]. Particularly in the context of the so called geometrothermodynamics [15,14], the geometrical relevant quantities, like the thermodynamic metric, are invariant with respect to Legendre transformations resembling the fact that the thermodynamic information does not depend on what fundamental relation (thermodynamic potential) is used. In this formalism, the representation invariance of the metric and its corresponding curvature scalar has been proved for simple thermodynamic systems [14]. On the other hand, inspired in fluctuation theory, a distance between points in a thermodynamic space can also be defined [11,12,16], and we can associate to this space a thermodynamic metric, a corresponding Riemann tensor and consequently a curvature scalar R. Both approaches coincide in the physical interpretation of the curvature scalar as a manifestation of the existence of intermolecular interactions. When the curvature associated to the corespondent thermodynamic metric is non-zero, an interaction of some nature is present [12,13], this is known as the curvature/interaction hypothesis. Other physical aspects that the scalar reveals, which has been proven for several thermodynamic systems, is the existence of first order phase transitions. The curvature scalar diverges at some point if a phase transition exists. For some systems, the point where the scalar diverges happens to be the critical point where the phase transition occurs [16, 14]. In the thermodynamic geometry of fluctuation theory, the sign of the curvature scalar also provides additional information. For some systems it is clear that the sign of R represents the kind of interaction, being attractive for a negative scalar and repulsive for a positive scalar [17]. The sign of R can also be associated to the bosonic or fermionic nature of the thermodynamic system, the Bose and Fermi ideal gases are a clear example of this, we have

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$R < 0$ in the first case and $R > 0$ in the second case [18,22]. For some other systems, it appears a change of sign in the curvature scalar, from negative to positive or the other way around. These cases generally appear where a different statistics, other than that of Boltzmann's, is considered [17,22]. Following the vast literature of the subject related to the thermodynamic geometry of the two approaches considered here, we find that the sign interpretation is more clear in the formalism of G. Ruppeiner [17] but even so, it is not at all clear that this interpretation could be valid for all thermodynamic systems.

In this work we particularly consider the curvature of a non-extensive ideal gas characterized by a generalized non-extensive entropy. The particular entropy we use depends only on the probability distribution and arises in the realm of superstatistics [1,6]. In order to get a better insight of the physics behind the curvature scalar of our thermodynamic system, we calculate the curvature scalar using the two formalisms mentioned earlier, we will call these two scalars, the geometrothermodynamic scalar for the scalar calculated following the formalism in [13] and the fluctuation theory scalar, to the scalar calculated following [17]. We will find that the particular entropy (statistics) we propose [1,6] modifies the geometric structure of the generalized thermodynamic space considered, namely a generalized ideal gas, giving rise to the appearance of an effective interaction.

The paper is organized as follows: First in section 2 we explain how our modified entropy, and its associated Boltzmann factor, arises by assuming a particular probability distribution. In section 3 we briefly introduce first the formalism of geometrothermodynamics developed by H. Quevedo [13] and describe how the thermodynamic metric is calculated. In this same section we also introduce the thermodynamic metric in the formalism of G. Ruppeiner [12]. We calculate the curvature scalar in both formalisms to further analyze and compare the thermodynamic information contained in the scalars using the interpretation of both formalisms. In section 4 we discuss the interpretation of both scalars and in section 5 we conclude and present the main results of our work.

2. Generalized entropies depending only on the probability distribution

The Boltzmann factor depending on the energy E of a microstate associated with a local cell of average temperature $1/\beta$ is given by

$$B(E) = \quad f(\beta)e^{-\beta E}d\beta \tag{1}$$

and different distributions $f(\beta)$ lead to different Boltzmann factors. Following the procedure stated in [2,4] it is possible, in principle, to associate a modified entropy to every Boltzmann factor. As an example we have that for the distribution $f(\beta) = \delta(\beta - \beta_0)$ the usual Boltzmann factor is recovered and from this, the Boltzmann–Gibbs entropy follows directly [4]. In [1] a Gamma distribution of the form

$$f_{p_l}(\beta) = \frac{1}{\beta_0 p_l \Gamma \quad \frac{1}{p_l}} \quad \frac{\beta}{\beta_0}\frac{1}{p_l} \quad ^{\frac{1-p_l}{p_l}} e^{-\beta/\beta_0 p_l}, \tag{2}$$

was proposed where, by maximizing the appropriate information measure, the parameter p_l can be identified with the probability and β_0 is the average inverse temperature. This distribution yields to the Boltzmann factor

$$B_{p_l}(E) = (1 + p_l\beta_0 E)^{-\frac{1}{p_l}}, \tag{3}$$

that leads to the following generalized entropy [1]

$$S = k \mathop{}_{l=1}^{\Omega} (1 - p_l^{p_l}). \tag{4}$$

It has been observed that when the fluctuations are small, the Boltzmann factor (3) can be approximated as an infinite sum where the first term is the usual Boltzmann factor and the first correction term seems to be the same even for different statistics [2]. It was shown in [21,19] that this is the case for the entropy in Eq. (4). We will further consider small fluctuations and we will take only the first correction term in entropy. Associated to this generalized entropy there is a generalized H function,

$$H = \quad d^3 p \quad e^{f \ln f} - 1 \quad , \tag{5}$$

it can be shown that it satisfies a generalized H-theorem [19]. Using a Maxwell distribution to calculate this new H function, keeping only the first order correction and the relation $H = -S/kV$, it follows

$$S_{eff} = -kN \quad \ln(n\lambda^3) - \frac{3}{2} \tag{6}$$
$$- \frac{kVn^2\lambda^3}{2^{5/2}} \quad \ln^2(n\lambda^3) - \frac{3}{2}\ln(n\lambda^3) + \frac{15}{16} \quad ,$$

where $\lambda = \frac{h}{\sqrt{2\pi mkT}}$ can be identified with the mean thermal wavelenght, k is the Boltzmann constant, V is the volume and T is the absolute temperature. The authors in [19] studied the thermodynamic properties of the corresponding generalized ideal gas. In this context, analysis of response functions shows a first correction having a universal form, that is, the same functional correction to all thermodynamic quantities derived from the generalized equations of state.

In order to obtain a thermodynamic potential, we assume that the conventional linear relation between internal energy and temperature holds. Within this approximation we obtain the following thermodynamic fundamental relation

$$S = kN\ln v + \frac{3kN}{2}\ln\frac{u}{b} + \frac{3kN}{2} \tag{7}$$
$$- \frac{kN}{2^{5/2}}\frac{b^{3/2}}{u^{3/2}v} \quad \ln^2 \quad \frac{b^{3/2}}{vu^{3/2}} \quad - \frac{3}{2}\ln \quad \frac{b^{3/2}}{vu^{3/2}} \quad + \frac{15}{16} \quad ,$$

where $u = \frac{U}{N}$, $v = \frac{V}{N}$ and $b = \frac{3h^2}{4\pi m}$. The first terms correspond to the usual entropy of the ideal gas, $S = kN\ln v + \frac{3kN}{2}\ln\frac{u}{b} + \frac{3kN}{2}$. We notice that the Sackur–Tetrode expression for the entropy of the ideal gas $S = kN\ln v + \frac{3kN}{2}\ln\frac{u}{b} + \frac{5kN}{2}$ can be recovered by an ad-hoc fixing term as it was originally proposed by Gibbs. It is not possible to recover the $5kN/2$ term from the classical calculation we made but this does not affect the further analysis which involves derivatives of the entropy, and this constant term does not affect the final result. At this point we have to clarify that the linear relation between internal energy and temperature that we have assumed makes our calculations to be more accurate for low densities or high temperatures and we will take this into account to make the interpretation of the behavior of the curvature scalars.

A previous thermodynamic analysis was made corresponding to a system characterized by a particular interaction. In [19] a system was considered of gas particles exposed to square-well and Lennard–Jonnes potentials. These potentials are well defined and a respective Boltzmann factor $B(E) = f(\beta, E, p_l)$ can be associated to these systems. A further analysis with Monte Carlo simulations

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