Duality in nonextensive statistical mechanics

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We revisit recent derivations of kinetic equations based on Tsallis' entropy concept. The method of kinetic functions is introduced as a standard tool for extensions of classical kinetic equations in the framework of Tsallis' statistical mechanics. Our analysis of the Boltzmann equation demonstrates a remarkable relation between thermodynamics and kinetics caused by the deformation of macroscopic observables.

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I. INTRODUCTION

The past decade has witnessed increasing interest in nonextensive statistical mechanics based on Tsallis' entropy concept [1,2]. Whereas most of the work has been done so far in the context of purely static consideration, more recently attempts have been made towards time-dependent processes out of equilibrium. In particular, in a recent paper [3], the authors have extended the classical Boltzmann equation in such a way as to obtain its analog for the case of Tsallis' entropy [1].

The motivation for this paper is that, in general, addressing the time-dependent processes may provide a test for certain postulated properties of static considerations. Specifically, we want to test consequences of definitions of macroscopic variables such as particle's density, momentum, and energy, in the way they are used in nonextensive thermodynamics. The outline and the main results of this paper are as follows: In the next section we recall, for the sake of completeness, the basic points of the nonextensive thermodynamics. In Sec. III, we revisit the transformation of the Boltzmann kinetic equation. Our analysis is based on the well-developed method of kinetic functions, and results are different from those of Ref. [3] only in some points inessential to our discussion. Equilibria in the kinetic picture are zeroes of the collision integral, and they can be found independently of any maximum entropy consideration. This gives us an opportunity to test which definitions of macroscopic variables should be taken in order to describe the same equilibrium states, also as the maximum entropy states. It is demonstrated that consistency rules out the deformed constraints. Instead, we find a relation between the two families of equilibria, one of which are nonextensive thermodynamic equilibria, the other is the equilibria of the kinetic equations. This relation, termed duality in the sequel, is given by the transform of Tsallis' nonextensivity parameter as $q'=2-q$. Some further implications of the duality are discussed.

II. THERMODYNAMICS

Let Γ be variables of a detailed description (phase variables), $f(\Gamma)$ distribution functions over the phase space, and $\boldsymbol{m}(\Gamma)$ microscopic observables (energy, momentum, etc.). Nonextensive thermodynamics [1,2] is based on two points:

(i) A set of concave functionals, S_q, $q>0$,

$$S_q=k(1-q)^{-1}\int [f(\Gamma)-f^q(\Gamma)]d\Gamma, \tag{1}$$

where integration over the phase space is replaced by summation in the discrete case. In the sequel, we use convex functionals $H_q=-k^{-1}S_q$, in order to save notation,

$$H_q=(1-q)^{-1}\int [f^q(\Gamma)-f(\Gamma)]d\Gamma. \tag{2}$$

The one-parametric family of functionals (2) can be considered as a continuous deformation of the classical Boltzmann-Gibbs-Shannon functional $H_1=\int F(\Gamma)\ln F(\Gamma)d\Gamma$, since $\lim_{q\to 1}H_q=H_1$. [This deformation is continuous, and differentiable but not continuously differentiable, the second derivative of the function $H_q(x)$ with respect to q at $q=1$ is divergent.]

(ii) Maximum entropy states, corresponding to the observables $\boldsymbol{m}$, are found as a solution to the problem,

$$S_q\to\max, \quad \int f d\Gamma=M_0, \quad \int \boldsymbol{m}f^q d\Gamma=\boldsymbol{M}. \tag{3}$$

The introduction of the nonlinear in f,q dependent constraints instead of the usual linear functionals, $\boldsymbol{M}=\int \boldsymbol{m}f d\Gamma$ is based on the following observation: Let $\{\lambda_0,\boldsymbol{\lambda}\}$ be Lagrange multipliers associated with constraints in the variational problem (3),

$$\delta S_q+\lambda_0\int \delta f d\Gamma+\boldsymbol{\lambda}\cdot\int \boldsymbol{m}f^{q-1}\delta f d\Gamma=0. \tag{4}$$

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Let $f^{(1)}(M_0,\boldsymbol{M})$ be the solution to the problem (3), and let $Z=\int f^{(1)}(1,\boldsymbol{M})d\Gamma$ be the partition function. Then, for each q, there exists a function

$$\ln_q(x)=\frac{x^{1-q}-1}{1-q}, \tag{5}$$

such that

$$\frac{\partial \ln_q Z}{\partial \boldsymbol{\lambda}}=\boldsymbol{M}. \tag{6}$$

This relation can be checked by inspection, and it provides a deformation of Gibbs' fundamental relation defining the free energy (or, in a broader sense, Jaynesian structure of thermodynamics). It is pertinent to mention here that this is a sufficient but not necessary deformation with a similar property. Indeed, also the use of the undeformed constraints,

$$S_q\rightarrow \max, \quad \int f d\Gamma=M_0, \quad \int \boldsymbol{m} f d\Gamma=\boldsymbol{M}, \tag{7}$$

satisfies the relation

$$\frac{\partial G_q}{\partial \boldsymbol{\lambda}}=\boldsymbol{M}. \tag{8}$$

Here G_q is the Legendre transform of the function

$$S_q^{(2)}(M_0,\boldsymbol{M})=S_q(f^{(2)}(M_0,\boldsymbol{M})).$$

The existence of the function G_q is guaranteed because the transform $f\rightarrow \delta S_q/\delta f$ is one into one. However, the important difference from the case (6) is that the explicit form of functions G_q is not known for a generic q and generic $\boldsymbol{m}$.

We discussed here only the formal aspect of the maximum entropy problem for a generic phase space Γ, and for a generic set of observables $\boldsymbol{m}$, without touching upon the question of existence of solutions to either problems (3) or (7). We shall come back to this point later on. Finally, whereas most of the standard sources on maximum entropy states are almost exclusively devoted to the Boltzmann-Gibbs-Shannon functional, this question has been studied in detail for a generic concave function S in the context of the master equation in Ref. [4].

III. KINETICS

A. Deformation of collision integral

Same as in Ref. [3], we focus our attention on the deformation of the Boltzmann collision integral. To this end, we use the following well known structure of the collision integral [5,4,6,7]: Let $f(\boldsymbol{v},\boldsymbol{x},t)$ be the one-particle distribution function, and H a strictly convex functional (associated concave functional, the entropy, is $S=-kH$). Let us denote $\mu=\delta H/\delta f$ the Volterra functional derivative of H. Then the following operator, $f\rightarrow Q(f)$, is defined as

$$Q=\int w(\boldsymbol{v}',\boldsymbol{v}_1'|\boldsymbol{v},\boldsymbol{v}_1)(e^{\mu_1'+\mu'}-e^{\mu_1+\mu})d\boldsymbol{v}_1'd\boldsymbol{v}'d\boldsymbol{v}_1. \tag{9}$$

Here we denote μ_1', μ', μ_1, and μ, the functional derivatives of H evaluated at $f(\boldsymbol{v}_1',\boldsymbol{x},t)$, $f(\boldsymbol{v}',\boldsymbol{x},t)$, $f(\boldsymbol{v}_1,\boldsymbol{x},t)$, and $f(\boldsymbol{v},\boldsymbol{x},t)$, respectively. The generalized function w gives the probability of scattering of the pair $(\boldsymbol{v}_1',\boldsymbol{v}')$ into $(\boldsymbol{v}_1,\boldsymbol{v})$, and it has the form

$$w=\omega(\boldsymbol{v}',\boldsymbol{v}_1'|\boldsymbol{v},\boldsymbol{v}_1)\,\delta(\boldsymbol{v}'+\boldsymbol{v}_1'-\boldsymbol{v}-\boldsymbol{v}_1) \times \delta(v'^2+v_1'^2-v^2-v_1^2). \tag{10}$$

The form of the function ω in this expression is known in the literature for various particle's interactions [9,10]. While a specific form of ω is unimportant to our discussion, we remind that it is derived from a purely mechanical consideration on the basis of Newton's equations of motion of two particles. This results in the well known symmetry of function ω (detail balance),

$$\omega(\boldsymbol{v}',\boldsymbol{v}_1'|\boldsymbol{v},\boldsymbol{v}_1)=\omega(\boldsymbol{v},\boldsymbol{v}_1|\boldsymbol{v}',\boldsymbol{v}_1'). \tag{11}$$

Various generalizations of the structure (9) can be found in the literature [4–7]. We recall the two formal features of the collision integral (9) valid for any H:

(i) The entropy production inequality for the entropy production $\sigma=\int(\delta S/\delta f)Q(f)d\boldsymbol{v}$,

$$\sigma=-\frac{k}{4}\int w(e^{\mu_1'+\mu'}-e^{\mu_1+\mu}) \times(\mu+\mu_1-\mu'-\mu_1')d\boldsymbol{v}_1'd\boldsymbol{v}'d\boldsymbol{v}_1d\boldsymbol{v}\geqslant 0. \tag{12}$$

(ii) Zero points of collision integral, $Q=0$, and zero points of entropy production, $\sigma=0$, satisfy

$$\mu^{\mathrm{eq}}=\mathrm{Lin}\{1,\boldsymbol{v},v^2\}, \tag{13}$$

where Lin denotes linear envelope.

Using any of the functionals H_q (2), and computing derivatives,

$$\mu_q=\delta H_q/\delta f=(1-q)^{-1}[1-qf^{q-1}], \tag{14}$$

together with Eq. (9), we obtain the desired family of collision integrals, $Q_q(f)$, and which provides a deformation of the Boltzmann collision integral. The latter is obtained in the limit of $q\rightarrow 1$.

Whereas all the general properties of the operator (9) are valid in the particular case H_q, we will write out explicitly Eqs. (13),(14) in terms of the equilibrium distribution function rather than the derivative of H_q in the equilibrium,

$$f_q^{\mathrm{eq}}=(a_0+\boldsymbol{a}_1\cdot\boldsymbol{v}+a_2v^2)^{1/(q-1)}, \tag{15}$$

where a_0, $\boldsymbol{a}_1$, and a_2 are arbitrary parameters.

B. Variational specification of equilibria

The analysis of the previous subsection is the result of a specification of the standard scheme (9) to H_q, and is only slightly different from Ref. [3]. This difference is due to the fact that Eq. (9) is based on the derivative of the H function whereas the authors [3] used a related quantity, $f^{q-1}\ln_q f$, and which is specific to the case (2). However, the most important feature of both the deformation is that *they make no attempt to alter the scattering probabilities w*, Eq. (10). Before going any further, we need a short reflection of the classical Boltzmann case.

In the classical Boltzmann's case, the (local) Maxwell distribution functions are described in three different ways. First, they are zero points of the collision integral. Second, they are zero points of the entropy production. Third, and final, they are maximizers of the entropy density under the linear constraints that fix the five hydrodynamic fields corresponding to the five collision invariants. In the classical case, the three sets of distribution functions, each set specified by one of the conditions just mentioned, are equivalent. Finally, it is only the third specification that equips the *set* of the local Maxwell distributions by a specific (thermodynamic) coordinate system (the density, the average velocity, and the temperature, the latter is in agreement with the fundamental thermodynamic relation).

This reminder is pertinent to our discussion because the two of the specifications (zeroes of the collision integral, and zeroes of the entropy production) are already fixed for the deformed Maxwell states (15) by adopting the form of the kinetic function, Eq. (9) and Eq. (10). Thus, we are led to the question, as to which is the third, variational specification of the set (15)? *A priori*, we have the two possibilities:

(i) Using the deformed constraints [problem (3)],

$$H_q \to \min, \quad \int \{1,\boldsymbol{v},v^2\} f^q d\boldsymbol{v} = \{M_0,\boldsymbol{M}_1,M_2\}. \tag{16}$$

(ii) Using the undeformed constraints [problem (7)],

$$H_q \to \min, \quad \int \{1,\boldsymbol{v},v^2\} f d\boldsymbol{v} = \{M_0,\boldsymbol{M}_1,M_2\}. \tag{17}$$

Solving formally both the problems by the method of Lagrange multipliers, we get

$$f_q^{\mathrm{eq}'} = (\alpha_0' + \boldsymbol{\alpha}_1' \cdot \boldsymbol{v} + \alpha_2')^{1/(1-q)}, \tag{18}$$

$$f_q^{\mathrm{eq}} = (\alpha_0 + \boldsymbol{\alpha}_1 \cdot \boldsymbol{v} + \alpha_2)^{1/(q-1)}, \tag{19}$$

for the problems (17) and (16), respectively. Obviously, if the deformation parameter q is fixed, and $q \neq 1$, it is the set (19) that stays in agreement with the two other specifications, Eq. (15). Thus, in the kinetic picture, consistency at $q \neq 1$ ultimatively requires the choice of the undeformed constraints for the variational specification. Several comments are in order.

(i) For infinite-dimensional systems such as the continuous Boltzmann equation, the moments of the local equilibria may not exist for some $q \neq 1$. This fact is also well known in the case of the classical Boltzmann equation: for example, the maximum entropy solution for the Boltzmann entropy does not exist if the observables are the density, the average momentum, the stress tensor, and the heat flux [11]. In such cases a regularization of divergent integrals is required. In particular, a regularisation by the argument that the magnitude of the microscopic velocity is restricted to the value dictated by finiteness of the *total* energy [11] seems relevant to our case. Another opportunity is to restore to a discretization in the velocity space (see, e.g., Ref. [12]).

(ii) If one insists on using deformed constraints for derivations of kinetic equations, then not only the collision integral but also the free flight operator must be deformed. Such derivations has to be based on the deformed Liouville equation. Let us recall that, if $U(\Gamma)$ is the particles' Hamiltonian, the classical Liouville equation conserves the energy, $E = \int U f d\Gamma$, any of the functionals S_q (1), but not the functionals $E_q = \int U f^q d\Gamma$. Therefore, the deformed Liouville equation has to read

$$\partial_t f = L \frac{\delta E_q}{\delta f}, \tag{20}$$

where L is the Poissonian operator. Obviously, dynamics (20) conserves the deformed energy E_q, as well as any of the functionals S_q. Development of the projection operator formalism to derive the deformed Boltzmann Eq. [13] is an interesting option left for a future work.

IV. DUALITY

The apparent discrepancy between the outcomes of the thermodynamics with the q-deformed constraints, and of the q-deformed kinetics is explained by the following duality: For each value of the deformation parameter q, there are two families of equilibrium distribution functions. The first (E family) F_q^E described by the maximizers of the entropy function S_q under q-deformed constraints. The second family (N family) F_q^N are stationary states of the deformed kinetics that are maximizers of the same entropy under the undeformed constraints. We have worked out explicitly the particular case of the Boltzmann equation, but the observation should be valid for any deformation of kinetics based on the kinetic function formalism. These families are related by the duality transform of the deformation parameter,

$$q' = 2 - q, \quad F_{q'}^E = F_q^N, \quad F_{q'}^N = F_q^E. \tag{21}$$

The Boltzmann-Gibbs-Shannon case is thereby characterized not just by the limiting feature at $q \to 1$ but also by self-duality: The only solution to the set of equations, $q' = q$, $q' = 2 - q$, is $q' = q = 1$. This is precisely the Boltzmann-Gibbs-Shannon limit of Tsallis' entropy family that in our presentation gives the identity of the E and of the N families of equilibria, $F_1^E = F_1^N$. This algebraic rather than the limiting description of the Boltzmann-Gibbs-Shannon case has not been mentioned before, to the best of our knowledge. Several concluding remarks are in order:

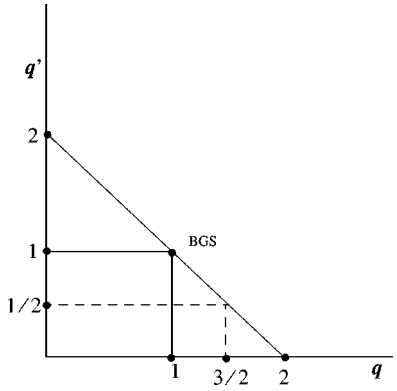

FIG. 1. Dual families F_q^E and F_q^N. BGS is the self-dual Boltzmann-Gibbs-Shannon limit.

(i) Deformation [3] also leads to the same result as ours, and, in fact, the transform $q'=2-q$ appears in an intermediate computation in Ref. [3]. However, the importance of this fact has not been mentioned by the authors.

(ii) Duality (21) selects the range of the deformation parameter q between 0 and 2. It is only in this range where both the E and the N families coexist. This is depicted in Fig. 1.

V. CONCLUSION

In this paper, we have analyzed the relation between the thermodynamic and kinetic description arising from the nonextensive statistical mechanics. We have argued that the well known formulation of kinetic models [4,5] provides a natural setup for such extensions. We have demonstrated this for the case of the Boltzmann collision integral. Several extensions of classical models are readily obtained in a straightforward way (for example, the deformation of the chemical kinetics that parallels the formulation of the Boltzmann equation, [7,8]). Based on this deformation, we were able to test which kind of maximum entropy principle is compatible with other properties of local equilibria. Finally, we have demonstrated that the intrinsic duality between thermodynamic and kinetic descriptions is present when the deformation parameter $q\neq 1$.

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