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Variational Method in Generalized Statistical Mechanics

by

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Abstract

Concavity properties of a recently generalized (not necessarily extensive) entropy enable, among others, the generalization of the Bogolyubov inequality, hence of the Variational Method in equilibrium Statistical Mechanics.

Key-words: Generalized entropy; Generalized statistical mechanics; Variational method; Bogolyubov inequality.

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Attempts to conveniently generalize the standard concept of entropy constitute an important concern in the Statistics literature [1]. Properties currently discussed in these works are *additivity* (or *extensivity*) and *subadditivity*. Curiously enough, no major interest is payed to *concavity*, which, from a physical point of view, is very important since it guarantees the thermodynamic stabilty of the system.

On a multifractal basis, a generalized entropy has been recently introduced with the aim of generalizing Statistical Mechanics [2] and Thermodynamics [3]. This new entropy has been the subject of much recent work [4–7] and can be regarded as a nonlogarithmic information measure. Moreover, it has enabled [8] the overcome of a longstanding puzzle in Astrophysics, namely, the inability of the Boltzmann-Gibbs statistics to provide a *finite* mass for the polytropic model of stellar dynamics [9] (we recall that the long range gravitational interaction between the stars of a galaxy makes the problem an intrinsically nonextensive one). This generalized entropy is given (in units of a conventional constant k) by [2]

$$S_q = \frac{1 - \sum_i p_i^q}{q-1} \tag{1}$$

where the set $\{p_i\}$ corresponds to a normalized probability distribution associated with the microscopic configurations of the system, and $q \in \Re$. A nondiagonal version of (1) reads [7]

$$S_q = \frac{Tr\hat{\rho}(1-\hat{\rho}^{q-1})}{q-1} \tag{2}$$

where $\hat{\rho}$ is the density operator (whose eigenvalues are $\{p_i\}$). It has been proven in [2] that, contrary to what happens with the well known Renyi entropy, S_q is concave (convex) for $q > 0$ ($q < 0$). For $q = 1$, S_q recovers the familiar Shannon entropy ($-Tr\hat{\rho}\ln\hat{\rho}$).

The aim of the present paper is to show that this concavity property allows for a natural extension, to arbitrary q, of the celebrated Bogolyubov inequality, hence of the Variational Method in equilibrium Statistical Mechanics.

Let us first consider the function $f(x) \equiv (1 - x^{q-1})/(q-1)$. It is straightforward to verify that, for $x \geq 0$,

$$f(x) \geq 1 - x \quad \text{if} \quad q < 2 \tag{3.a}$$

$$= 1 - x \quad \text{if} \quad q = 2 \tag{3.b}$$

$$\leq 1 - x \quad \text{if} \quad q > 2 \tag{3.c}$$

It follows that, for $q < 2$,

$$Tr\hat{\rho}_0 \left[\frac{1-(\frac{\hat{\rho}}{\hat{\rho}_0})^{q-1}}{q-1}\right] \geq Tr\rho_0 \left(1 - \frac{\rho}{\rho_0}\right) = 1 - 1 = 0 \tag{4}$$

where $\hat{\rho}$ and $\hat{\rho}_0$ are arbitrary density operators (the equality holds if and only if $\hat{\rho} = \hat{\rho}_0$). If we consider all possible values of q, we obtain

$$\frac{1-<(\hat{\rho}/\hat{\rho}_0)^{q-1}>_0}{q-1} \equiv Tr\hat{\rho}_0\left[\frac{1-(\frac{\hat{\rho}}{\hat{\rho}_0})^{q-1}}{q-1}\right] \geq 0 \quad \text{if} \quad q<2 \tag{5.a}$$

$$= 0 \quad \text{if} \quad q=2 \tag{5.b}$$

$$\leq 0 \quad \text{if} \quad q>2 \tag{5.c}$$

In the $q \rightarrow 1$ limit, $(\hat{\rho}/\hat{\rho}_0)^{q-1} \sim 1+(q-1)\ln(\hat{\rho}/\hat{\rho}_0)$, hence, Eq. (5.a) implies the well known inequality [10]

$$-Tr\rho_0 \ln \rho_0 \leq -Tr\rho_0 \ln \rho \tag{6}$$

We see that, for $q \neq 1$, Eqs. (5) cannot be split in two pieces, as in Eq. (6). This is, of course, a consequence of the nonextensivity of S_q.

Eqs. (5) pave the way for the extension of Bogolyubov inequality. Let $\hat{\mathcal{H}}$ and $\hat{\mathcal{H}}_0$ stand for two arbitrary Hamiltonians, one of which ($\hat{\mathcal{H}}_0$) is of a manageable nature, whereas the other ($\hat{\mathcal{H}}$) is not easy to handdle, although it is precisely the one in which we are primarily interested. Associated with these Hamiltonians, we have the follwoing equilibrium density operators [3]

$$\hat{\rho}_0 = [1-\beta(1-q)\hat{\mathcal{H}}_0]^{\frac{1}{1-q}}/Z_0 \tag{7}$$

with

$$Z_0 \equiv Tr[1-\beta(1-q)\hat{\mathcal{H}}_0]^{\frac{1}{1-q}} \tag{8}$$

and

$$\hat{\rho} = [1-\beta(1-q)\hat{\mathcal{H}}]^{\frac{1}{1-q}}/Z \tag{9}$$

with

$$Z \equiv Tr[1-\beta(1-q)\hat{\mathcal{H}}]^{\frac{1}{1-q}} \tag{10}$$

where $\beta \equiv 1/kT$. Let us recall that $\hat{\rho}_0$ vanishes ($\hat{\rho}$ vanishes) whenever the eigenvalues of $[1-\beta(1-q)\hat{\mathcal{H}}_0]$ ($[1-\beta(1-q)\hat{\mathcal{H}}]$) vanish or are negative [2]. By replacing Eqs. (7) and (9) into (5) we obtain

$$\frac{1-H\,\frac{Z^{1-q}}{Z_0^{1-q}}}{q-1} \geq 0 \quad \text{if} \quad q<2 \tag{11.a}$$

$$= 0 \quad \text{if} \quad q=2 \tag{11.b}$$

$$\leq 0 \quad \text{if} \quad q>2 \tag{11.c}$$

with

$$H \equiv < \frac{1-\beta(1-q)\hat{\mathcal{H}}_0}{1-\beta(1-q)\hat{\mathcal{H}}} >_0 \tag{12}$$

The free energies associated respectively with $\mathcal{H}_0$ and $\mathcal{H}$ are given by [3]

$$F_0 = -\frac{1}{\beta}\,\frac{Z_0^{1-q}-1}{1-q} \tag{13}$$

and

$$F = -\frac{1}{\beta}\,\frac{Z^{1-q}-1}{1-q} \tag{14}$$

With the help of Eqs. (13) and (14) we can now cast the left member of Eqs. (11) into the form

$$\frac{1 - H\,\frac{1-\beta(1-q)F}{1-\beta(1-q)F_0}}{q-1} \tag{15}$$

Finally, we can rewrite Eqs. (11) as follows

$$\begin{aligned} F &\leq \frac{F_0}{H} + \left(1-\frac{1}{H}\right)\frac{1}{\beta(1-q)} \quad \text{if} \quad q<2 && (16.a)\\ &= \frac{F_0}{H} - \left(1-\frac{1}{H}\right)\frac{1}{\beta} \quad \text{if} \quad q=2 && (16.b)\\ &\geq \frac{F_0}{H} + \left(1-\frac{1}{H}\right)\frac{1}{\beta(1-q)} \quad \text{if} \quad q>2 && (16.c)\end{aligned}$$

where we have used the fact that both $[1-\beta(1-q)F_0]$ and $[1-\beta(1-q)F]$ are positive. In the $q \to 1$ limit we have

$$H \sim 1 + \beta(1-q) < \hat{\mathcal{H}} - \hat{\mathcal{H}}_0 >_0 \tag{17}$$

hence

$$F \leq F_0 + < \hat{\mathcal{H}} - \hat{\mathcal{H}}_0 >_0 \tag{18}$$

which is the well known [10] Bogolyubov inequality.

Inequalities (16) legitimate the use of parameters entering $\hat{\mathcal{H}}_0$ as variational ones in order to discuss the complex Hamiltonian $\mathcal{H}$. In other words, it is justified to extremalize the right-hand side of (16). This is of course the basis of the Variational Method in equilibrium Statistical Mechanics, which is now generalized to arbitrary q on account of the concavity properties of S_q.

Notice also in definition (12) that a ratio appears rather than the customary difference $(\mathcal{H} - \mathcal{H}_0)$. This again shows that lack of extensivity is not essential in order to attempt physical applications. On the other hand, lack of concavity, a property which is sometimes disregarded by the Statistics community, would preclude the use, in Physics, of this type of variational procedures.

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