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1993 J. Phys. A: Math. Gen. 26 L893

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J. Phys. A: Math. Gen. 26 (1993) L893–L896. Printed in the UK

LETTER TO THE EDITOR

Variational method in generalized statistical mechanics

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Received 12 May 1993

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.

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 stability 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 non-logarithmic information measure. Moreover, it has enabled [8] a longstanding puzzle in astrophysics to be overcome, namely, the inability of 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 non-extensive 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 $q \in \mathscr{R}$. A non-diagonal version of (1) reads [7]

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

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 ($-\mathrm{Tr}\,\hat{\rho}\ln\hat{\rho}$).

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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 $x\geqslant 0$,

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

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

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

It follows that, for $q<2$,

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

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

$$\frac{1-\langle(\hat{\rho}/\hat{\rho}_0)^{q-1}\rangle_0}{q-1}\equiv \mathrm{Tr}\,\hat{\rho}_0\left[\frac{1-(\hat{\rho}/\hat{\rho}_0)^{q-1}}{q-1}\right]\geqslant 0 \quad \text{if } q<2 \tag{5a}$$

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

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

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

$$-\mathrm{Tr}\,\rho_0\ln\rho_0\leqslant -\mathrm{Tr}\,\rho_0\ln\rho. \tag{6}$$

We see that, for $q\neq 1$, equations (5) cannot be split in two pieces, as in equation (6). This is, of course, a consequence of the non-extensivity of S_q.

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

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

with

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

and

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

with

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

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

$$\frac{1-H(Z^{1-q}/Z_0^{1-q})}{q-1}\geqslant 0 \quad \text{if } q<2 \tag{11a}$$

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

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

with

$$H\equiv\left\langle\frac{1-\beta(1-q)\hat{\mathscr{H}}_0}{1-\beta(1-q)\hat{\mathscr{H}}}\right\rangle_0. \tag{12}$$

The free energies associated, respectively, with $\mathscr{H}_0$ and $\mathscr{H}$ 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 (13) and (14) we can now cast the left member of (11) into the form

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

Finally, we can rewrite (11) as follows:

$$F\leqslant\frac{F_0}{H}+\left(1-\frac{1}{H}\right)\frac{1}{\beta(1-q)} \quad \text{if } q<2 \tag{16a}$$

$$=\frac{F_0}{H}-\left(1-\frac{1}{H}\right)\frac{1}{\beta} \quad \text{if } q=2 \tag{16b}$$

$$\geqslant\frac{F_0}{H}+\left(1-\frac{1}{H}\right)\frac{1}{\beta(1-q)} \quad \text{if } q>2 \tag{16c}$$

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

$$H\approx 1+\beta(1-q)\langle\hat{\mathscr{H}}-\hat{\mathscr{H}}_0\rangle_0 \tag{17}$$

hence

$$F\leqslant F_0+\langle\hat{\mathscr{H}}-\hat{\mathscr{H}}_0\rangle_0 \tag{18}$$

which is the well known [10] Bogolyubov inequality.

Inequalities (16) legitimate the use of parameters entering $\hat{\mathscr{H}}_0$ as variational ones in order to discuss the complex Hamiltonian $\mathscr{H}$. 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 $(\mathscr{H} - \mathscr{H}_0)$. 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.

The authors are indebted to E M F Curado and R N Silver for interesting remarks. One of us (AP) wishes to thank the CBPF for its kind hospitality.

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