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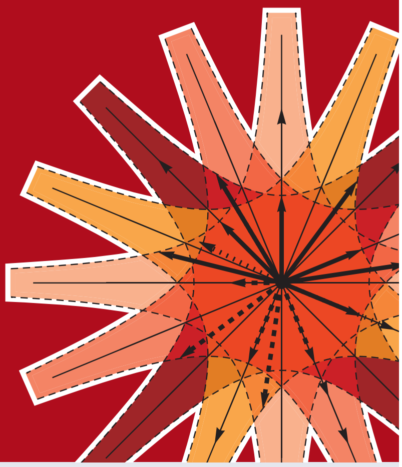

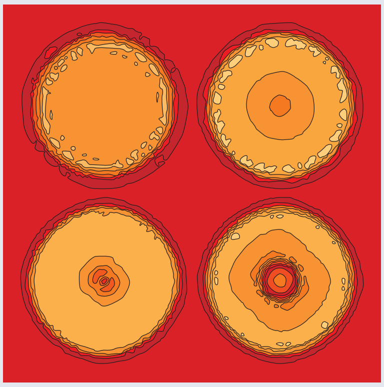

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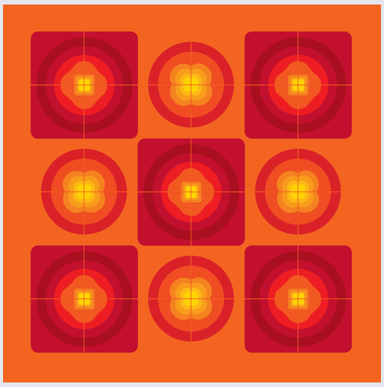

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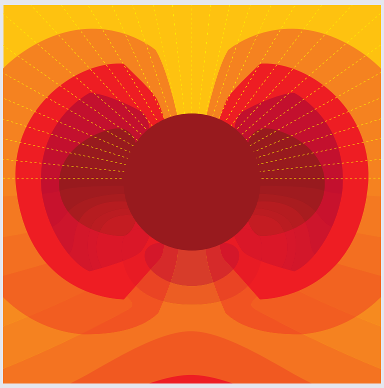

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Comment

Comment on "Possible divergences in Tsallis' thermostatistics" by Plastino A. and Rocca M. C.

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The nonextensive statistical mechanics introduced by Tsallis [1] and developed over the last 25 years by numerous researchers [2] is based on a generalization of the Boltzmann entropy,

$$S_q = \frac{1}{q-1}\left(1-\sum_n p_n^q\right) \rightarrow \frac{1}{q-1}\left(1-\int p^q(x)\,\mathrm{d}x\right) \underset{q\to 1}{\Rightarrow} -\int p(x)\log p(x)\,\mathrm{d}x, \quad (1)$$

where we have given the expressions for both discrete and continuous variables. Statistical mechanics is then developed using the maximum entropy formalism whereby the probabilities are determined by maximizing the entropy subject to the constraint of constant average energy and normalizability of the distribution function. The result is a so-called q-exponential distribution

$$p_n = Z_q^{-1}\exp_q\left(\beta\left(\varepsilon_n - U\right)\right) \equiv Z_q^{-1}\left(1-(1-q)\,Z_q^{q-1}\beta\left(\varepsilon_n - U\right)\right)_+^{\frac{1}{1-q}}, \quad (2)$$

where Z_q is determined by normalization, β is the inverse temperature, ε_n is the energy of state n, U is the average total energy and the notation $(x)_+^y$ means x^y when $x>0$ and zero otherwise. The expression for the continuous case is analogous. In both cases, the distribution becomes the usual exponential, Maxwell-Boltzmann distribution in the limit $q \to 1$. The present authors noted that for Hamiltonian systems [3], the continuous distribution is only normalizable for values of the parameter q satisfying $0 \le q \le 1 + \frac{2}{ND}$, where N is the number of particles and D the dimension of the system. Since it is the case that $q>1$ corresponds to so-called fat-tailed distributions observed in many physical and non-physical systems (see Part III in [2]) and so is of most interest, this places a significant constraint on the utility of the formalism for many-body systems ($N \gg 1$). The divergence of the normalization results from the combination of the power-law distribution (2) and the unbounded nature of the kinetic energy [3].

Recently, Plastino and Rocca [4] have proposed a modification of the Tsallis formalism that is intended to circumvent this problem. They note that in the usual, Boltzmann-Gibbs, statistical mechanics, the normalization factor, or partition function[1], can be written in the form

$$Z_{q=1} = \int_0^\infty e^{-\beta U} g(U)\mathrm{d}U, \qquad g(U) \equiv \int \delta(U - H(\Gamma))\mathrm{d}\Gamma, \quad (3)$$

where $H(\Gamma)$ is the Hamiltonian (assumed to be shifted so as to be bounded below by zero) and Γ represents a point in phase space. So, the partition function can be viewed as a Laplace transform of the density of states. Similarly, the average of any function of the Hamiltonian, $\langle f(H)\rangle$, can be written in a similar form with the replacement of $g(U)$ by $f(U)\,g(U)$: in particular, this applies to the average

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[1] We note that Plastino and Rocca (PR) identify the normalization factor with the partition function without comment. Although it is not our main point, this cannot be correct since the normalization factor has dimensions and the partition function should be dimensionless. In the usual formulation, there is an additional factor of $\frac{1}{h^{DN}N!}$ relating these quantities where h is Planck's constant. We will follow PR in ignoring this distinction.

energy and to the entropy. What is proposed in [4] is to eliminate the divergences by replacing the Laplace transform structure by the so-called q-Laplace transform [5] defined for an arbitrary function $f(x)$ as

$$\widetilde{f}_q(\alpha) \equiv \Theta(\mathrm{Re}(\alpha)) \times \sum_n a_n \int_0^\infty x^n \left(1-(1-q)\alpha x^{n(q-1)}\right)^{\frac{1}{1-q}} \mathrm{d}x, \qquad (4)$$

where it is assumed that the function $f(x)$ can be expanded about $x = 0$ with coefficients a_n (in fact, the expression given above is the sum of the q-Laplace transforms of individual terms x^n but this distinction is not important). Hence, the proposed partition function is $Z_q = \widetilde{g}_q(\beta)$, with similar expressions for the energy and entropy. It is then shown that for a harmonic oscillator these expressions are all finite.

A careful examination of the procedure developed in [4] raises several problems which makes it questionable as a basis for statistical mechanics:

1) While this procedure yields a finite value for the partition function Z_q (eq. (23) in [4]), the original distribution $f_q \sim \exp_q(-\beta(H-U))$ remains un-normalizable (beyond the domain $0 \leq q \leq 1+\frac{2}{ND}$). It therefore fails to address the fundamental problem with the nonextensive Tsallis formalism. Introducing the q-Laplace prescription only "cures" averages of functions of the energy.

2) If the "partition function" is not related to the normalization of the distribution, we assume its finiteness is only important because it is related to the free energy in the usual way. Indeed, in this modified formalism, one still finds that $U - TSZ_q^{1-q} = -k_B T \ln Z_q$ so that this should be identified as the free energy. However, in this case the modified free energy and internal energy do not satisfy the thermodynamic relation $U = (\partial\beta F/\partial\beta)_V$.

3) It is stated in the third section of [4] that in the nonextensive approach the corresponding values for the partition function, the mean energy, and the entropy can be obtained by replacing the quantities appearing in the classical statistical thermodynamics expressions by their q-analogues[2]. Now the resulting "entropy" is not equivalent to the original Tsallis entropy evaluated with the q-exponential distribution (compare eqs. (15) and (21) of ref. [4]). Nor is it an alternative to the Tsallis entropy since it is not a *functional* of the distribution but in fact only applies to the distribution derived from maximization of the Tsallis entropy. What is the justification for using the Tsallis entropy to determine the distribution but another "entropy" to define the thermodynamics?

4) The expansion used in eq. (4) above seems quite arbitrary. One could, for example, replace $a_n x^n$ by $(2^n a_n)\left(\frac{x}{2}\right)^n$ and thereby obtain an inequivalent form for the function $\widetilde{f}_q(\alpha)$. In fact, this problem is evident in the proposed thermodynamic expressions since they involve quantities of the form $\beta U^{n(q-1)+1}$ which should be dimensionless but are not. One can "solve" this problem by replacing $a_n U^n$ by $b_n\left(\frac{U}{u}\right)^n$ with u a constant having the dimensions of energy and $b_n \equiv u^{-n}a$ but the results then depend on the choice of u.

In conclusion, we have analyzed the proposal of a modified formulation of nonextensive statistical thermodynamics based on the use of the q-Laplace transform in order to eliminate divergences related to the non-normalizability of the q-distribution function introduced in [1]. While the modifications proposed in [4] do indeed produce finite quantities, the fundamental problem of the divergence of the normalization of the q-distribution function remains unsolved and it is unclear whether the new formulation can produce a consistent thermodynamics.

* * *

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[2] Note however that the expression given for the entropy, eq. (11) of ref. [4], differs from the Tsallis definition where the first factor of P is raised to the power q.