Possible divergences in Tsallis’ thermostatistics

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Abstract – Lutsko and Boon have shown via elegant theoretical reasoning (EPL, 95 (2011) 20006), that Tsallis’ thermostatistics is affected by divergence problems. We explicitly verify such fact in trying to compute the nonextensive \( q \)-partition function for the harmonic oscillator in more than two dimensions. One can see that it indeed diverges. The appeal to the so-called \( q \)-Laplace transform, where the \( q \)-exponential function plays the role of the ordinary exponential, is seen to overcome the serious problem envisaged by Lutsko and Boon.

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Introduction. – Divergences are quite important in theoretical physics. Indeed, the study and elimination of divergences of a physical theory is perhaps one of the most important branches of theoretical physics. The quintessential typical example is the attempt to quantify the gravitational field, which so far has not been achieved. Some examples of elimination of divergences can be seen in ref. [1–5].

Now, the so-called \( q \)-exponential function [6],

\[
\begin{align*}
\epsilon_q(x) &= \left[ 1 + (1 - q)x \right]^{1/(1-q)}; \\
q \in \mathbb{R}; \quad \epsilon_q(x) &\to e^x \text{ when } q \to 1,
\end{align*}
\]

(1)

is the flagship of nonextensive statistics (NET) (see [6] and references therein), a subject that has captured the interest of literally hundreds of researchers, that have produced several thousand papers in such respect in the last years [7]. They explore via NET the fact that natural phenomena and laboratory experiments yield a wide spectrum of empiric results demonstrating data-distributions clearly deviating from exponential decay [6,7]. Nonextensive statistical mechanics is an approach that explains this non-Boltzmann behavior using deformed exponential distributions (such as \( q \)-exponentials exhibiting long tails when \( q > 1 \)). These distributions are empirically encountered in a variety of scientific disciplines. One can mention subjects as variegated as turbulence, cosmic rays, earthquake’s magnitudes distributions, speed distributions in bacterial populations, geological, nuclear, particle, cosmic phenomena, financial market data, polymers, EEG analysis, Vlasov equations, etc. (see, for instance, [6–11]).

Moreover, the \( \epsilon_q \)-functions are the natural solutions to an interesting new version of the nonlinear Schrödinger equation (NLSE), recently advanced by Nobre, Rego-Monteiro and Tsallis [12,13] (see also [14]). This NLSE constitutes an intriguing proposal that is part of a program to investigate nonlinear versions of some of the basic equations of physics, a research venue that registers significant activity [15,16]. Here we show that, when regarded as a probability distribution function, the \( q \)-exponential leads to a divergent partition function in two or more dimensions, which constitutes a potential catastrophe for \( q \)-nonextensivity, with several thousands of papers referring to it in the last 15 years.

One should mention that Boon and Lutsko [17,18] have already shown, in two interesting papers, that divergences exist in Tsallis’ thermo-statistics in some classical settings. What we discuss here is how to avoid these divergences in Tsallis’ theory both for the harmonic oscillator and in the general case of a well-behaved Hamiltonian. Our main idea revolves around the concept of energy density, central in statistical mechanics, as seen for example in the classical text-book by Reif [19].

Partition function for the Harmonic Oscillator (HO). – Using appropriate units, the partition function of the \( n \)-dimensional harmonic oscillator is

\[
Z = \int_{-\infty}^{\infty} e^{-\beta \left( p^2 + Q^2 \right)} d^n p \, d^n q,
\]

(2)

where \( P^2 = p_1^2 + p_2^2 + \cdots p_n^2 \), \( Q^2 = q_1^2 + q_2^2 + \cdots q_n^2 \).
Taking into account that i) the value of a solid angle in the \( n \)-dimensional \( p \)-space and \( q \)-space is (see [20]) \( \Omega_p = \Omega_q = 2\pi^{n/2}/\Gamma(n/2) \), ii) performing the change of variables \( P^2 + Q^2 = U \), \( Q = \sqrt{U - P^2} \), and iii) using the result
\[
\int_0^u x^{\nu-1}(u-x)^{\mu-1} \, dx = u^{\mu+\nu-1} \text{B}(\mu, \nu),
\]
where \( \text{B} \) is Euler’s Beta function \([21]\), we obtain for \( Z \)
\[
Z = \frac{\pi^n}{\Gamma(n)} \int_0^\infty U^{n-1} e^{-\beta U} \, dU,
\]
\( U \) being the HO energy and \( g(U) = [\pi^n/\Gamma(n)]U^{n-1} \) the associated energy density.

It is of the essence to note that the partition function can also be obtained as the Laplace transform of the energy density \([22]\).

Following a similar line of reasoning to that leading to (4), we obtain for the mean energy \( \mathcal{U} \) and the entropy \( \mathcal{S} \)
\[
\mathcal{U} = \int_{-\infty}^{\infty} \left( P^2 + Q^2 \right) e^{-\beta P^2 + \beta Q^2} \frac{d^np \, d^nq}{Z} \Rightarrow \quad (5)
\]
\[
\mathcal{U} = \frac{\pi^n}{\Gamma(n)Z} \int_0^\infty U^n e^{-\beta U} \, dU, \quad \text{and} \quad \quad (6)
\]
\[
\mathcal{S} = \frac{\pi^n}{\Gamma(n)Z} \int_0^\infty (\ln Z + \beta U)U^{n-1} e^{-\beta U} \, dU. \quad \quad (7)
\]

**Divergences in Tsallis’ theory.** — Lutsko and Boon have discussed divergences in Tsallis’ theory \([17,18]\). We demonstrate the same below in what we believe is a more direct, straightforward, and explicit fashion. In the nonextensive (Tsallis’) approach the corresponding values for the \( q \)-partition function \( Z_q \), the mean energy \( \mathcal{U} \), and the Tsallis’ entropy \( \mathcal{S} \) are obtained using \([6]\): i) the \( q \)-exponential function of energy instead of the exponential function and ii) the \( q \)-logarithm function in place of the logarithmic function. One has, for the probability,
\[
P_q[H(p, x)] = \frac{e_q[-\beta H(p, x)]}{Z_q},
\]
with \( \ln_q x = \frac{x^{1-q} - 1}{1-q} \to \ln x \) for \( q \to 1 \).

One then finds
\[
Z_q = \frac{\pi^n}{\Gamma(n)Z_q} \int_0^\infty U^{n-1} [1 + (q-1)\beta U]^{1/2-q} \, dU, \quad (13)
\]
where the real parameter \( q \) obeys \( 1 < q < 2 \), and
\[
\mathcal{U} = \frac{\pi^n}{\Gamma(n)Z_q} \int_0^\infty U^n [1 + (q-1)\beta U]^{1/2-q} \, dU, \quad (14)
\]
\[
\mathcal{S} = \left\{ \frac{\pi^n (Z_q^{1-q} - 1)}{\Gamma(n)Z_q^{q-1}} \int_0^\infty U^{n-1} [1 + (q-1)\beta U]^{1/2-q} \, dU + \frac{\pi^n \beta}{\Gamma(n)Z_q^{2-q}} \int_0^\infty U^n [1 + (q-1)\beta U]^{1/2-q} \, dU \right\}. \quad (15)
\]

Looking at (13), we immediately detect a serious problem: the partition-defining integral diverges for \( q \geq 3/2 \) and \( n \geq 2 \). For example, if \( q = 3/2 \) and \( n = 2 \) we have
\[
Z_q = \frac{\pi^n}{\Gamma(n)Z_q} \int_0^\infty U^{n-1} \left[ 1 + \frac{\beta U}{2} \right]^{-2} \, dU, \quad (16)
\]
which is clearly divergent. For the average energy the situation is even worse.

For \( q \geq 3/2 \) and \( n \geq 1 \) we see that the integral is divergent, even in the one-dimensional case.

Moreover for \( q = 5/4 \) and \( n \geq 3 \) we obtain
\[
\mathcal{U} = \frac{\pi^n}{\Gamma(n)Z_q} \int_0^\infty U^n \left[ 1 + \frac{\beta U}{2} \right]^{-4} \, dU. \quad (17)
\]
This integral is divergent. The integral (15) registers a similar pitfall. We wish to make it clear here that if one were to set a \( q \)-bound, as for example, \( q \leq 3/2 \) or \( q \leq 5/4 \), this would not quite solve the problem of eliminating the divergences of the theory, as these depend on several factors. These are: i) the dimension of the pertinent space and ii) the joint behavior of the partition function and the average energy.

**Solution via \( q \)-Laplace transforms of the energy density \([23]\).** — The origin of these divergences that, as we have just demonstrated, plague Tsallis’ theory, can be accurately pinpointed. It is well known (cf. (4)) that \( Z \) is the Laplace transform of the energy density. Thus, (13) should be the \( q \)-Laplace transform \([23]\) (that replaces the \( q \)-exponential function) of the energy density, but this is not so. Accordingly, the correct way of obtaining a \( Z_q \) should pass through the \( q \)-Laplace Transform of the energy density, as explained at length in \([23]\).
In ref. [23] one sees that the expression for the unilateral $q$-Laplace transform of a function $f(U)$, belonging to a special set $\Omega_f$ defined in [23], reads

$$L(\beta, q) = H[\mathcal{R}(\beta)]\int f(U)(1 - (1 - q)\beta U)f(U)^{(q - 1)} \frac{dU}{U},$$

(18)

where $H$ is the Heaviside function and the brackets correspond to the argument of the $q$-Laplace transform, that will play a leading role below, for the special function $f(U) = U^{n-1}$. Consequently, $Z_q$ should be evaluated via

$$Z_q = \frac{\pi^n}{\Gamma(n)} \int_0^\infty U^{n-1}[1 + (q - 1)\beta U^{n(q-1)+1}] \frac{dU}{U},$$

(19)

and, in a similar fashion, for $U$ and $S$ one should have the expressions

$$U = \frac{\pi^n}{\Gamma(n)Z_q} \int_0^\infty U^n[1 + (q - 1)\beta U^{n(q-1)+1}] \frac{dU}{U},$$

(20)

$$S = \left\{ \frac{\pi^n[Z_q^{n-1} - 1]}{\Gamma(n)Z_q^{q}(1 - q)} \times \int_0^\infty U^{n-1}[1 + (q - 1)\beta U^{n(q-1)+1}] \frac{dU}{U} \right. \left. + \frac{\pi^n\beta}{\Gamma(n)Z_q^q} \int_0^\infty U^n[1 + (q - 1)\beta U^{n(q-1)+1}] \frac{dU}{U} \right\}.$$  

(21)

Integral (19) can be evaluated making the change of variable $x = U^{(n-1)(q-1)+1}$ and using (see ref. [24])

$$\int_0^\infty \frac{x^{\mu - 1}}{(1 + \beta x)^\nu} dx = \beta^{-\mu}B(\mu, \nu - \mu),$$

(22)

that leads us to find for $Z_q$ a convergent expression, namely,

$$Z_q = \left\{ \frac{\pi^n[\beta(q - 1)]^{-\frac{n-1}{q-1}}}{\Gamma(n)[(n - 1)(q - 1) + 1]} \times B \left[ \frac{n}{(n - 1)(q - 1) + 1}, \frac{1}{q - 1}, \frac{n}{n(q - 1) + 1} \right] \right\},$$

(23)

Analogously, we find convergent expressions for $U$ and $S$ and

$$U = \left\{ \frac{\pi^n[\beta(q - 1)]^{-\frac{n+1}{q-1}}}{\Gamma(n)Z_q[n(q - 1) + 1]} \times B \left[ \frac{n+1}{n(q - 1) + 1}, \frac{1}{q - 1}, \frac{n+1}{n(q - 1) + 1} \right] \right\},$$

(24)

$$S = \left\{ \frac{\pi^n[Z_q^{n-1} - 1][\beta(q - 1)]^{-\frac{n+1}{q-1}}}{\Gamma(n)Z_q^{2n-1}(1 - q)} \times B \left[ \frac{n}{(n - 1)(q - 1) + 1}, \frac{1}{q - 1}, \frac{n}{n(q - 1) + 1} \right] \right\},$$

(25)

We appreciate thus that the use of the $q$-Laplace transform of the energy density makes all $q$-thermodynamics’ variables to be finite.

**The general case.** – In the general case of a non-singular Hamiltonian which depends on $2n$ variables $p_1, p_2, \ldots, p_n$ and $q_1, q_2, \ldots, q_n$ we have

$$Z = \int_{-\infty}^{\infty} e^{-\beta H(p, q)} d^n p d^n q.$$  

(26)

We assume that the Hamiltonian is bounded from below. Appealing, for example, to the change of variables $U = H(p, q) - E_{\text{min}}$, so that one can write

$$q_i = g(U, p_1, \ldots, p_n, q_1, \ldots, q_n),$$

we obtain for $Z$

$$Z = e^{-\beta E_{\text{min}}} \int_{-\infty}^{\infty} e^{-\beta U} dU \times \int_{-\infty}^{\infty} J(U, p, q_1, \ldots, q_{i-1}, q_{i+1}, \ldots, q_n) d^n p d^n q,$$  

(27)

where $J$ is the Jacobian of the change of variables that yields an “energy density”. We then obtain for this energy density $f$ the expression

$$f(U) = \int_{-\infty}^{\infty} J(U, p, q_1, \ldots, q_{i-1}, q_{i+1}, \ldots, q_n) d^n p d^n q.$$  

(28)

Thus, $Z$ can be written in the form

$$Z = e^{-\beta E_{\text{min}}} \int_0^\infty f(U) e^{-\beta U} dU.$$  

(29)

Analogously we obtain for $U$ and $S$

$$U = E_{\text{min}} + e^{-\beta E_{\text{min}}} \int_0^\infty f(U) e^{-\beta U} dU.$$  

(30)

$$S = e^{-\beta E_{\text{min}}} \ln Z + \beta E_{\text{min}} e^{-\beta E_{\text{min}}} \int_0^\infty f(U) e^{-\beta U} dU + e^{-\beta E_{\text{min}}} \beta \int_0^\infty f(U) e^{-\beta U} dU.$$  

(31)
we are entitled to write

\[ f(U) = \sum_{n=0}^{\infty} a_n U^n, \]  

and obtain the convergent result

\[ Z = e^{-\beta E_{\text{min}}} \sum_{n=0}^{\infty} a_n \int_0^\infty U^n e^{-\beta U} \, dU, \]  

\[ U = E_{\text{min}} + \frac{e^{-\beta E_{\text{min}}}}{Z} \sum_{n=0}^{\infty} a_n \int_0^\infty U^{n+1} e^{-\beta U} \, dU, \]  

\[ S = e^{-\beta E_{\text{min}}} \frac{\ln Z + \beta E_{\text{min}}}{Z} \sum_{n=0}^{\infty} a_n \int_0^\infty U^n e^{-\beta U} \, dU \]

\[ + e^{-\beta E_{\text{min}}} \frac{\beta}{Z} \sum_{n=0}^{\infty} a_n \int_0^\infty U^{n+1} e^{-\beta U} \, dU. \]  

Taking into account the nonlinearity of the q-Laplace transform, from (33),(34), and (35) we obtain, adapting things to the nonextensive, q-scenario with \( E_{\text{min}} \geq 0 \),

\[ Z_q = [1 + \beta (q-1)E_{\text{min}}] \frac{1}{Z_q} \]

\[ \times \sum_{n=0}^{\infty} a_n \int_0^\infty U^n [1 + (q-1)\beta U^{n(q-1)+1}]^{\frac{1}{1-q}} \, dU \]  

\[ U = \left\{ E_{\text{min}} + \frac{[1 + \beta (q-1)E_{\text{min}}]}{Z_q} \right\} \frac{1}{Z_q} \]

\[ \times \sum_{n=0}^{\infty} a_n \int_0^\infty U^{n+1} [1 + (q-1)\beta U^{(n+1)(q-1)+1}]^{\frac{1}{1-q}} \, dU \]  

\[ S = \left\{ \frac{1}{Z_q} \left( Z_q^{1-q} - 1\right) \right\} \frac{1}{Z_q} \]

\[ \times \sum_{n=0}^{\infty} a_n \int_0^\infty U^n [1 + (q-1)\beta U^{n(q-1)+1}]^{\frac{1}{1-q}} \, dU \]

\[ + \frac{\beta}{Z_q} \left[ 1 + \beta (q-1)E_{\text{min}} \right] \frac{1}{Z_q} \]

\[ \times \sum_{n=0}^{\infty} a_n \int_0^\infty U^{n+1} [1 + (q-1)\beta U^{(n+1)(q-1)+1}]^{\frac{1}{1-q}} \, dU \]  

and attain convergence in every instance. Similar formulas are valid for \( E_{\text{min}} \leq 0 \). Note that the entropy satisfies the usual relation for Tsallis’ entropy:

\[ S = Z_q^{q-1} \ln Z_q + \beta U. \]  

Note that, so as to obtain the entropy (38) we have started our considerations from the Tsallis entropy definitions and then we proceeded with our q-Laplace transform.

The essence of our maneuvers was to replace the q-exponential by the argument of the q-Laplace transform. Thus, the center of gravity is displaced from probability distributions to energy densities. Note that the latter are well-established empirical quantities characterizing a given system, while the interpretation of the former is a matter of controversy, as, for instance, Bayesian vs. frequentist. Thus, this shifting is empirically sound.

**Conclusions.** – It is well known that, for obtaining the partition function \( Z \), two alternative routes can be followed:

- the “natural” one, given by \( Z \)'s definition and
- \( Z \) as the Laplace transform of the energy density.

In the orthodox Boltzmann-Gibbs instance, that uses the ordinary exponential function, the two routes yield the same result.

We have here proved that such is not the case for Tsallis’ thermostatistics, for which the first alternative diverges in three or more dimensions, due to the long tail of the q-exponential function. One must necessarily follow the second path, that yields finite results. Thus, the q-Laplace transform becomes an indispensable tool for nonextensive statistics.

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REFERENCES

[1] **BOLLINI C. G. and GIAMBIAJGI J. J., Phys. Lett. B**, 40 (1972) 566; **Nuovo Cimento B**, 12 (1972) 20.

[2] **BOLLINI C. G. and GIAMBIAJGI J. J., Phys. Rev. D**, 53 (1996) 5761.

[3] "t HOOF T. G. and VELTMAN M., *Nucl. Phys. B*, 44 (1972) 189.

[4] **BOLLINI C. G., ESCOBAR T. and ROCCA M. C., Int. J. Theor. Phys., 38** (1999) 2315.

[5] **BOLLINI C. G. and ROCCA M. C., Int. J. Theor. Phys., 43** (2004) 59; 1019; **46** (2007) 3030.

[6] **GELL-MANN M. and TSALLIS C. (Editors), Nonextensive Entropy: Interdisciplinary applications**, (Oxford University Press, Oxford) 2004; **TSALLIS C., Introduction to Nonextensive Statistical Mechanics: Approaching a Complex World** (Springer, New York) 2009.

[7] See **http://tsallis.cat.cbpf.br/biblio.htm** for a regularly updated bibliography on the subject.

[8] MA WEN-JONG and **HU CHIN-KUN, J. Phys. Soc. Jpn., 79** (2010) 024005.

[9] MA WEN-JONG and **HU CHIN-KUN, J. Phys. Soc. Jpn., 79** (2010) 024006.
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[10] CAPURRO A., DIAMBRA L., LORENZO D., MACADAR O., MARTIN M. T., MOSTACCIO C. and PLASTINO A., Physica A, 257 (1998) 149.
[11] PLASTINO A. R. and PLASTINO A., Braz. J. Phys., 29 (1999) 79.
[12] NOBRE F. D., REGO-MONTEIRO M. A. and TSALLIS C., Phys. Rev. Lett., 106 (2011) 140601.
[13] NOBRE F. D., REGO-MONTEIRO M. A. and TSALLIS C., EPL, 97 (2012) 41001.
[14] CURILEF S., PLASTINO A. R. and PLASTINO A., Physica A, 392 (2013) 2631; TORANZO I. V., PLASTINO A. R., DEHESA J. S. and PLASTINO A., Physica A, 392 (2013) 3945.
[15] SCOTT A. C., The Nonlinear Universe (Springer, Berlin) 2007.
[16] SULEM C. and SULEM P. L., The Nonlinear Schrodinger Equation: Self-Focusing and Wave Collapse (Springer, New York) 1999.
[17] BOON J. P. and LUTSKO J. F., Phys. Lett. A, 375 (2011) 329.
[18] LUTSKO J. F. and BOON J. P., EPL, 95 (2011) 20006.
[19] REIF F., Fundamentals of Statistical and Thermal Physics (McGraw-Hill, New York) 1965.
[20] GUELFAND I. M. and CHILOV G. E., Les Distributions, Vol. 1 (Dunod, Paris) 1962.
[21] GRADSHTEYN I. S. and RIZHIK I. M., Table of Integrals Series and Products (Academic Press, New York) 1965, p. 284, 3.191.1.
[22] ROMANINI D. and LEHMANN K. K., J. Chem. Phys., 98 (1993) 6437.
[23] PLASTINO A. and ROCCA M. C., Physica A, 392 (2013) 5581.
[24] GRADSHTEYN I. S. and RIZHIK I. M., Table of Integrals Series and Products (Academic Press, New York) 1965, p. 284, 3.194.3.