Possible Divergences in Tsallis' Thermostatistics

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Abstract

Trying to compute the nonextensive q-partition function for the Harmonic Oscillator in more than two dimensions, one encounters that it diverges, which poses a serious threat to Tsallis' thermostatistics. Appeal to the so called q-Laplace Transform, where the q-exponential function plays the role of the ordinary exponential, is seen to save the day.

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1 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 references [1, 2, 3, 4, 5].

The so-called q-exponential function [6]

$$\begin{gathered} e_q(x) = [1 + (1-q)x]_+^{1/(1-q)}; \\ q \in \mathcal{R};\ e_q(x) \rightarrow e^x \text{ when } q \rightarrow 1, \end{gathered} \tag{1}$$

is the flagship of non-extensive statistics (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]. Indeed, natural phenomena and laboratory experiments yield a wide spectrum of empiric results demonstrating data-distributions clearly deviating from exponential decay [6, 7]. Non-extensive statistical mechanics is an approach that explains this non-Boltzmann behavior, with 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, and cosmic phenomena, or financial market data [6, 7].

Moreover, the e_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 [8, 9] (see also [10]). This NLSE constitutes an intriguing proposal that is part of a program to investigate non-linear versions of some of the basic equations of physics, a research venue that registers significant activity [11, 12]. 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 [13, 14] 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 [15].

2 Partition Function for the Harmonic Oscillator (HO)

Using appropriate units, the partition function of n-dimensional harmonic oscillator is

$$\mathcal{Z} = \int\limits_{-\infty}^{\infty} e^{-\beta(P^2+Q^2)}\ d^np\ d^nq \tag{2}$$

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 n-dimensional p-space and q-space is (see [16]) $\Omega_p = \Omega_q = 2\pi^{n/2}/\Gamma(n/2)$, ii) performing the change of variables $P^2 + Q^2 = U$ $Q = \sqrt{U - P^2}$, and iii) using the result

$$\int\limits_0^u x^{\nu-1}(u-x)^{\mu-1}\ dx = u^{\mu+\nu-1}\mathcal{B}(\mu,\nu), \tag{3}$$

where $\mathcal{B}$ is the Euler's Beta function [17], we obtain for $\mathcal{Z}$

$$\mathcal{Z} = \frac{\pi^n}{\Gamma(n)} \int_0^\infty U^{n-1} e^{-\beta U} \, dU, \tag{4}$$

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 [18].

Following a similar line of reasoning to that leading to (4), we obtain for the *mean energy* $\mathcal{U}$ and the entropy S

$$\mathcal{U} = \int_{-\infty}^{\infty} (P^2 + Q^2) \frac{e^{-\beta(P^2+Q^2)}}{\mathcal{Z}} \, d^n p \, d^n q \quad \Rightarrow \tag{5}$$

$$\mathcal{U} = \frac{\pi^n}{\Gamma(n)\mathcal{Z}} \int_0^\infty U^n e^{-\beta U} \, dU, \quad \text{and} \tag{6}$$

$$\mathcal{S} = \frac{\pi^n}{\Gamma(n)\mathcal{Z}} \int_0^\infty (\ln \mathcal{Z} + \beta U) U^{n-1} e^{-\beta U} \, dU. \tag{7}$$

3 Divergences in Tsallis' Theory

Lutsko and Boon have discussed divergences in Tsallis' theory [13, 14]. 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 $\mathcal{Z}_q$, 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,

$$P_q[H(p,x)] = \frac{e_q[-\beta H(p,x)]}{\mathcal{Z}_q}, \tag{8}$$

where

$$\mathcal{Z}_q = \int e_q[-\beta H(p,x)] \, d^n p d^n x, \tag{9}$$

while the mean energy is

$$\mathcal{U} = \int H(p,x) P_q[H(p,x)] \, d^n p d^n x, \tag{10}$$

and the entropy:

$$S = -\int P_q[H(p,x)] \ln_q P_q[H(p,x)]\; d^n p d^n x, \tag{11}$$

with

$$\ln_q x = \frac{x^{1-q}-1}{1-q} \;\to \ln x \quad for \quad q \to 1 \tag{12}$$

One then finds

$$\mathcal{Z}_q = \frac{\pi^n}{\Gamma(n)} \int\limits_0^\infty U^{n-1}[1+(q-1)\beta U]^{\frac{1}{1-q}}\; dU, \tag{13}$$

where the real parameter q obeys $1 < q < 2$, and

$$\mathcal{U} = \frac{\pi^n}{\Gamma(n)\mathcal{Z}_q} \int\limits_0^\infty U^n[1+(q-1)\beta U]^{\frac{1}{1-q}}\; dU, \tag{14}$$

$$\mathcal{S} = \left\{ \frac{\pi^n(\mathcal{Z}_q^{1-q}-1)}{\Gamma(n)\mathcal{Z}_q^{2-q}(1-q)} \int\limits_0^\infty U^{n-1}[1+(q-1)\beta U]^{\frac{1}{1-q}}\; dU + \right.$$

$$\left. \frac{\pi^n \beta}{\Gamma(n)\mathcal{Z}_q^{2-q}} \int\limits_0^\infty U^n[1+(q-1)\beta U]^{\frac{1}{1-q}}\; dU \right\}. \tag{15}$$

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 $n \geq 2$ we have

$$\mathcal{Z}_q = \frac{\pi^n}{\Gamma(n)} \int\limits_0^\infty U^{n-1} \left[1+\frac{\beta U}{2}\right]^{-2}\; dU, \tag{16}$$

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.

For example for $q = 3/2$ and $n \geq 1$ we obtain:

$$\mathcal{U} = \frac{\pi^n}{\Gamma(n)} \int\limits_0^\infty U^n \left[1+\frac{\beta U}{2}\right]^{-2}\; dU, \tag{17}$$

This integral is divergent. The integral (15) registers a similar pitfall.

4 Solution via q-Laplace Transforms of the energy density [19]

The origin of these divergences that, as we have just demonstrated, plague Tsallis' theory, is clear. It is well known (Cf. (4)) that $\mathcal{Z}$ is the Laplace Transform of the energy density. Thus, (13) should be the q-Laplace Transform [19] (that replaces the q-exponential function) of the energy density, but this is not so. Accordingly, the correct way of obtaining a $\mathcal{Z}_q$ should pass through the q-Laplace Transform of the energy density, as explained at length in [19].

In reference [19] one sees that the expression for the unilateral q-Laplace transform of a function $f(U) \in \Omega_I$ reads

$$L(\beta, q) = H[\Re(\beta)] \int\limits_0^\infty f(U)\{1-(1-q)\beta U[f(U)]^{(q-1)}\}^{\frac{1}{1-q}}\, dU, \tag{18}$$

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* $f(U) = U^{n-1}$ (for a definition of Ω_I see [19]). Consequently, $\mathcal{Z}_q$ should be evaluated via

$$\mathcal{Z}_q = \frac{\pi^n}{\Gamma(n)} \int\limits_0^\infty U^{n-1}[1+(q-1)\beta U^{(n-1)(q-1)+1}]^{\frac{1}{1-q}}\, dU, \tag{19}$$

and, in similar fashion, for $\mathcal{U}$ and $\mathcal{S}$ one should have the expressions

$$\mathcal{U} = \frac{\pi^n}{\Gamma(n)\mathcal{Z}_q} \int\limits_0^\infty U^n[1+(q-1)\beta U^{n(q-1)+1}]^{\frac{1}{1-q}}\, dU, \tag{20}$$

$$\mathcal{S} = \left\{ \frac{\pi^n(\mathcal{Z}_q^{1-q}-1)}{\Gamma(n)\mathcal{Z}_q^{2-q}(1-q)} \times \right.$$

$$\int\limits_0^\infty U^{n-1}[1+(q-1)\beta U^{(n-1)(q-1)+1}]^{\frac{1}{1-q}}\, dU$$

$$\left. + \frac{\pi^n\beta}{\Gamma(n)\mathcal{Z}_q^{2-q}} \int\limits_0^\infty U^n[1+(q-1)\beta U^{n(q-1)+1}]^{\frac{1}{1-q}}\, dU \right\}. \tag{21}$$

Integral (19) can be evaluated making the change of variable $x = U^{(n-1)(q-1)+1}$ and using (see Ref. [20])

$$\int\limits_0^\infty \frac{x^{\mu-1}}{(1+\beta x)^\nu}\, dx = \beta^{-\mu}\mathcal{B}(\mu, \nu-\mu), \tag{22}$$

that leads us to find for $\mathcal{Z}_q$ a convergent expression, namely,

$$\mathcal{Z}_q = \left\{ \frac{\pi^n [\beta(q-1)]^{-\frac{n}{(n-1)(q-1)+1}}}{\Gamma(n)[(n-1)(q-1)+1]} \times \right.$$

$$\left. \mathcal{B}\left[\frac{n}{(n-1)(q-1)+1}, \frac{1}{q-1} - \frac{n}{(n-1)(q-1)+1}\right] \right\}. \tag{23}$$

Analogously, we find convergent expressions for U and S

$$\mathcal{U} = \left\{ \frac{\pi^n [\beta(q-1)]^{-\frac{n+1}{n(q-1)+1}}}{\Gamma(n)\mathcal{Z}_q[n(q-1)+1]} \times \right.$$

$$\left. \mathcal{B}\left[\frac{n+1}{n(q-1)+1}, \frac{1}{q-1} - \frac{n+1}{n(q-1)+1}\right] \right\} \tag{24}$$

and

$$\mathcal{S} = \left\{ \frac{\pi^n (\mathcal{Z}_q^{1-q}-1)[\beta(q-1)]^{-\frac{n}{(n-1)(q-1)+1}}}{\Gamma(n)\mathcal{Z}_q^{2-q}(1-q)[(n-1)(q-1)+1]} \times \right.$$

$$\left. \mathcal{B}\left[\frac{n}{(n-1)(q-1)+1}, \frac{1}{q-1} - \frac{n}{(n-1)(q-1)+1}\right] \right\} +$$

$$\left\{ \frac{\pi^n \beta [\beta(q-1)]^{-\frac{n+1}{n(q-1)+1}}}{\Gamma(n)\mathcal{Z}_q^{2-q}[n(q-1)+1]} \times \right.$$

$$\left. \mathcal{B}\left[\frac{n+1}{n(q-1)+1}, \frac{1}{q-1} - \frac{n+1}{n(q-1)+1}\right] \right\} \tag{25}$$

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

5 The General Case

In the general case of a Hamiltonian which depends on $2n$ variables $p_1, p_2, ..., p_n$ and $q_1, q_2, ..., q_n$ we have

$$\mathcal{Z} = \int\limits_{-\infty}^{\infty} e^{-\beta H(p,q)}\ d^n p\ d^n q \tag{26}$$

Appealing, for example, to the change of variables $U = H(p,q)$,

$q_i = g(U, p_1, ..., p_n, q_1, ..., q_{i-1}, q_{i+1}, ..., q_n)$ we obtain for $\mathcal{Z}$

$$\mathcal{Z} = \int\limits_{0}^{\infty} e^{-\beta U}\ dU \int\limits_{-\infty}^{\infty} J(U, p, q_1, ..., q_{i-1}, q_{i+1}, ..., q_n)\ d^n p\ d^{n-1} q. \tag{27}$$

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

$$f(U) = \int_{-\infty}^{\infty} J(U, p, q_1, ..., q_{i-1}, q_{i+1}, ..., q_n)\ d^n p\ d^{n-1} q. \tag{28}$$

Thus, $\mathcal{Z}$ can be written in the form:

$$\mathcal{Z} = \int_0^{\infty} f(U) e^{-\beta U}\ dU. \tag{29}$$

Analogously we obtain for $\mathcal{U}$ and S

$$\mathcal{U} = \frac{1}{\mathcal{Z}} \int_0^{\infty} U f(U) e^{-\beta U}\ dU. \tag{30}$$

$$S = \frac{1}{\mathcal{Z}} \int_0^{\infty} (\ln \mathcal{Z} + \beta U) f(U) e^{-\beta U}\ dU. \tag{31}$$

Considering that for a well behaved Hamiltonian $f(U)$ *is an analytic function in the upper right quadrant of the complex plane* we are entitled to write

$$f(U) = \sum_{n=0}^{\infty} a_n U^n, \tag{32}$$

and obtain the convergent result

$$\mathcal{Z} = \sum_{n=0}^{\infty} a_n \int_0^{\infty} U^n e^{-\beta U}\ dU, \tag{33}$$

$$\mathcal{U} = \frac{1}{\mathcal{Z}} \sum_{n=0}^{\infty} a_n \int_0^{\infty} U^{n+1} e^{-\beta U}\ dU, \tag{34}$$

$$S = \frac{1}{\mathcal{Z}} \ln \mathcal{Z} \sum_{n=0}^{\infty} a_n \int_0^{\infty} U^n e^{-\beta U}\ dU + \frac{\beta}{\mathcal{Z}} \sum_{n=0}^{\infty} a_n \int_0^{\infty} U^{n+1} e^{-\beta U}\ dU. \tag{35}$$

Taking into account the nonlinearity of the q-Laplace transform, from (33),(34), and (35) we obtain, *adapting things to the nonextensive, q-scenario*,

$$\mathcal{Z}_q = \sum_{n=0}^{\infty} a_n \int_0^{\infty} U^n [1 + (q-1)\beta U^{n(q-1)+1}]^{\frac{1}{1-q}}\ dU, \tag{36}$$

$$\mathcal{U}_q = \frac{1}{\mathcal{Z}_q} \sum_{n=0}^{\infty} a_n \int_0^{\infty} U^{n+1} [1 + (q-1)\beta U^{(n+1)(q-1)+1}]^{\frac{1}{1-q}} \, dU, \tag{37}$$

$$\mathcal{S} = \left\{ \frac{\mathcal{Z}_q^{1-q} - 1}{\mathcal{Z}_q^{2-q}(1-q)} \sum_{n=0}^{\infty} a_n \int_0^{\infty} U^n [1 + (q-1)\beta U^{n(q-1)+1}]^{\frac{1}{1-q}} \, dU \right.$$
$$\left. + \frac{\beta}{\mathcal{Z}_q^{2-q}} \sum_{n=0}^{\infty} a_n \int_0^{\infty} U^{n+1} [1 + (q-1)\beta U^{(n+1)(q-1)+1}]^{\frac{1}{1-q}} \, dU \right\}, \tag{38}$$

and attain convergence in every instance. Note that having i) a partition function, ii) a mean energy and iii) an entropy, we automatically get a thermostatistics. This may not be the orthodox one, but is quite a legitimate one nonetheless.

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 later 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.

6 Conclusions

It is well known that, for obtaining the partition function $\mathcal{Z}$, two alternative routes can be followed:

- the "natural" one, given by $\mathcal{Z}$'s definition and
- $\mathcal{Z}$ 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] C. G. Bollini and J. J. Giambiagi: Phys. Lett. **B 40**, (1972), 566.Il Nuovo Cim. **B 12**, (1972), 20.

[2] C. G. Bollini and J.J Giambiagi : Phys. Rev. **D 53**, (1996), 5761.

[3] G.'t Hooft and M. Veltman: Nucl. Phys. **B 44**, (1972), 189.

[4] C. G. Bollini, T. Escobar and M. C. Rocca : Int. J. of Theor. Phys. **38**, (1999), 2315.

[5] C. G Bollini and M.C. Rocca : Int. J. of Theor. Phys. **43**, (2004), 59. Int. J. of Theor. Phys. **43**, (2004), 1019. Int. J. of Theor. Phys. **46**, (2007), 3030.

[6] M. Gell-Mann and C. Tsallis, Eds. *Nonextensive Entropy: Interdisciplinary applications*, Oxford University Press, Oxford, 2004; C. Tsallis, *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] F.D. Nobre, M A. Rego-Monteiro and C. Tsallis, Phys. Rev. Lett **106** (2011) 140601.

[9] F.D. Nobre, M.A. Rego-Monteiro, and C. Tsallis, Europhysics Letters 97 (2012) 41001.

[10] S. Curilef, A.R. Plastino, A. Plastino, Physica A **392** (2013) 2631; I. V. Toranzo, A. R. Plastino, J. S. Dehesa, A. Plastino, Physica A **392** (2013) 3945.

[11] A.C. Scott, *The Nonlinear Universe* (Springer, Berlin, 2007).

[12] C. Sulem and P.L. Sulem, *The Nonlinear Schrodinger Equation: Self-Focusing and Wave Collapse* (Springer, New York, 1999).

[13] J. P. Boon and J. F. Lutsko: Phys. Lett. A **375**, (2011), 329.

[14] J. F. Lutsko and J. P. Boon: Europhys. Lett. **95**, (2011), 20006.

[15] F. Reif, *Fundamentals of statistical and thermal physics* (McGraw-Hill, NY, 1965).

[16] I. M. Guelfand and G. E. Chilov, *Les Distributions*, Vol. 1 (Dunod, Paris, 1962).

[17] I. S. Gradshteyn and I. M. Rizhik, *Table of Integrals Series and Products* (Academic Press, NY, 1965, p.284, **3.191**,1).

[18] D. Romanini and K. K. Lehmann, J. Chem. Phys. **98** (1993) 6437.

[19] A. Plastino, M.C.Rocca, Physica A **392** (2013) 5581.

[20] I. S. Gradshteyn and I. M. Rizhik, *Table of Integrals Series and Products* (Academic Press, NY, 1965, p.284, **3.194**,3).