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On The Problem of Constraints In Nonextensive Formalism: A Quantum Mechanical Treatment

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Relative entropy (divergence) of Bregman type recently proposed by T. D. Frank and Jan Naudts is considered and its quantum counterpart is used to calculate purity of the Werner state in nonextensive formalism. It has been observed that Bregman type divergence is suitable for q>1 whereas Csiszàr type is suitable for q∈ $(0, 1)$. It is then argued that the difference is due to the fact that the relative entropy of Bregman type is related to the first choice thermostatistics whereas the one of Csiszàr type is related to the third choice thermostatistics. Moreover, it has been noted that these two measures show different qualitative behavior with respect to F due to the fact that these divergences being written compatible with different constraints. The possibility of writing a relative entropy of Bregman type compatible with the third choice has been investigated further. The answer turns out to be negative as far as the usual transformation from ordinary probabilities to the escort probabilities are considered.

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I. INTRODUCTION

A nonextensive generalization of the standard Boltzmann-Gibbs (BG) entropy has been proposed by C. Tsallis in 1988 [1-4]. This new definition of entropy is given by

$$S_q = k\frac{1-\sum_{i=1}^{W} p_i^q}{q-1}, \tag{1}$$

where k is a positive constant which becomes the usual Boltzmann constant in the limit q→ 1, p_i is the probability of the system in the ith microstate, W is the total number of the configurations of the system.The entropic index q is a real number, which characterizes the degree of nonextensivity as can be seen from the following pseudo-additivity rule:

$$S_q(A+B)/k = [S_q(A)/k] + [S_q(B)/k] + (1-q)[S_q(A)/k][S_q(B)/k], \tag{2}$$

where A and B are two independent systems i.e., p_{ij}(A+B)=$p_i(A)$$p_j(B)$. As q→ 1, the nonextensive entropy definition in Eq. (1) becomes

$$S_{q\to 1} = -k_B \sum_{i=1}^{W} p_i \ln p_i, \tag{3}$$

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which is the usual BG entropy. This means that the definition of nonextensive entropy contains BG statistics as a special case. The cases q <1, q >1 and q = 1 correspond to superextensivity, subextensivity and extensivity, respectively.

The nonextensive formalism is used in systems with long-ranged interactions, long-ranged memories, and systems which evolve in fractal-like space-time. Even though BG statistics can be used successfully in investigating extensive systems, physical systems such as Euler two-dimensional turbulence [5], high energy collisions [6-9], nematic liquid crystals [10], stellar polytropes [11], the nonisotropic rigid rotator model [12] and Fokker-Planck systems [13,14] can be given as examples for which the nonextensive formalism has been used successfully.

From a mathematical point of view, the nonextensive formalism is being formulated by using the q-deformed logarithm and q-deformed exponential which can be given, respectively, as

$$\ln_q x \equiv \frac{x^{1-q}-1}{1-q} \qquad\qquad \exp_q x \equiv [1+(1-q)x]^{1/(1-q)}. \tag{4}$$

These functions become the usual logarithmic and exponential functions as q→ 1. Moreover, other functions in common use can be generalized in a similar manner. For example q-sine function [15] can be defined as

$$\mathrm{Si}\, n_q x \equiv \sum_{j=0}^{\infty} \frac{(-1)^j Q_{2j} x^{2j+1}}{(2j+1)!}, \tag{5}$$

where the function $\mathrm{Q}_n(q)$ is given by

$$Q_n(q) \equiv 1.q.(2q-1).(3q-2)...[nq-(n-1)]. \tag{6}$$

J. Naudts [16-19] generalized the idea of q-deformed exponentials and logarithms to what is now called $\kappa-$deformed exponentials i.e., $\exp_\kappa(x)$. A $\kappa-$deformed exponential is a convex function with a value of one when its argument is zero. It is also equal to or greater than zero for all real arguments. The $\kappa-$deformed logarithm is defined in a similar manner. By choosing a $\kappa-$deformed logarithm as

$$\ln_\kappa(x) = (1+\frac{1}{\kappa})(x^\kappa - 1) \qquad\qquad -1 < \kappa < 1, \tag{7}$$

and its inverse function as

$$\exp_\kappa(x) = [1+\frac{\kappa}{1+\kappa}x]_+^{1/\kappa}, \tag{8}$$

where $[x]_+ = \max\{0, x\}$, one immediately obtains the nonextensive formalism by setting κ equal to (q-1). For $\kappa = 0$, they become the usual logarithmic and exponential function respectively.

Likewise, if one chooses for the deformed exponential

$$\exp_\kappa(x) = [\kappa x + \sqrt{1+\kappa^2 x^2}]^{1/\kappa} \qquad -1 < \kappa < 1 \text{ and } \kappa \neq 0, \tag{9}$$

and the deformed logarithm as

$$\ln_\kappa(x) = \frac{1}{2\kappa}(x^\kappa - x^{-\kappa}), \tag{10}$$

one obtains Kaniadakis'deformed functions [20]. Again, in the limit $\kappa = 0$, these functions coincide with the usual logarithmic and exponential functions. In the sense emphasized above, both of the Tsallis and Kaniadakis formalisms can be explained within the scheme of deformed functions approach proposed by Jan Naudts.

In Section II, we use quantum divergences in the nonextensive formalism in order to calculate the purity of state in the case of Werner states. We show that each of them provides us with a different answer. This difference is resolved by considering the first and third choices of internal energy constraint. Our final observation is related to the fact that there is no nonextensive relative entropy expression of Bregman type which is compatible with third choice of constraint. We summarize the results in Section III.

II. RELATIVE ENTROPIES, FIDELITY AND CONSTRAINTS

One particularly important concept is the one of relative entropy: In extensive statistics, the physical meaning of relative entropy is the free energy difference. In addition to this, it plays a very decisive role in the context of the second law of thermodynamics in the nonextensive formalism. Indeed, Abe and Rajagopal showed that there might be expected a violation of the second law if the nonextensive index q is not in the range (0,2] [21]. To be able to do this, they made use of the nonextensive relative entropy definition of Csiszár type [22]

$$I_q(\rho \parallel \sigma) = \frac{1}{q-1}\ [Tr(\rho^q \sigma^{1-q}) - 1]. \tag{11}$$

Recently, J. Naudts [18] and T. D. Frank [14, 23] gave an alternative definition of relative entropy of Bregman type [24] which reads

$$D_q(\rho \parallel \sigma) = \frac{1}{q-1}\ [Tr(\rho^q) - Tr(\rho\sigma^{q-1})] - [Tr(\rho\sigma^{q-1}) - Tr(\sigma^q)]. \tag{12}$$

S. Abe [25] made use of Eq. (11) in order to calculate the purity of Werner state in the nonextensive framework. For this purpose, he used Werner state [26] which is given by the density matrix

$$\rho_W = F \mid \Psi^-\rangle\langle\Psi^- \mid + \frac{1-F}{3}(\mid \Psi^+\rangle\langle\Psi^+ \mid + \mid \Phi^+\rangle\langle\Phi^+ \mid + \mid \Phi^-\rangle\langle\Phi^- \mid), \quad \frac{1}{4} \le F \le 1 \tag{13}$$

where

$$\mid \Psi^\pm\rangle \equiv \frac{1}{\sqrt{2}}(\mid +-\rangle \pm \mid -+\rangle), \tag{14}$$

and

$$\mid \Phi^\pm\rangle \equiv \frac{1}{\sqrt{2}}(\mid ++\rangle \pm \mid --\rangle). \tag{15}$$

F is the fidelity of ρ_W with respect to the pure reference state $\sigma =\mid \Psi^-\rangle\langle\Psi^- \mid$. For the time being, we restrict ourselves to the interval q$\in (0,1)$ since Eqs. (11) and (12) should not be too sensitive to small eigenvalues of the matrices as in Ref [25]. If we substitute Werner states in order to find the degree of purity with respect to σ in Eq.(11), we obtain

$$I_q(\rho_W \parallel \mid \Psi^-\rangle\langle\Psi^- \mid) = \frac{1}{1-q}(1-F^q). \tag{16}$$

Indeed, this is the result already obtained by Abe in Ref. [25]. Let us consider the alternative definition of quantum divergence proposed by Naudts and T. D. Frank in Eq. (12) and repeat the above calculation by substituting σ, as defined earlier. First, let us consider the first two terms on the right hand side of Eq. (12)

$$Tr(\rho^q - \rho\sigma^{q-1}) = \sum_i \langle i \mid (\rho^q - \rho\sigma^{q-1}) \mid i\rangle, \tag{17}$$

$$= Tr(\rho^q) - \langle\Psi^- \mid \rho \mid \Psi^-\rangle. \tag{18}$$

For the second term, we have

$$Tr(\rho\sigma^{q-1} - \sigma^q) = \sum_i \langle i \mid (\rho\sigma^{q-1} - \sigma^q) \mid i\rangle = \langle \Psi^- \mid \rho \mid \Psi^-\rangle - \langle \Psi^- \mid \Psi^-\rangle. \tag{19}$$

Summing all the terms above, we obtain

$$D_q(\rho \parallel \sigma) = \frac{1}{q-1}\ [Tr(\rho^q) - \langle \Psi^- \mid \rho \mid \Psi^-\rangle] - \langle \Psi^- \mid \rho \mid \Psi^-\rangle + \langle \Psi^- \mid \Psi^-\rangle. \tag{20}$$

Next, we make use of Werner states ρ_W instead of the generic ρ in the expression above and obtain

$$D_q(\rho \parallel \sigma) = \frac{1}{q-1}\ [F^q + 3(\frac{1-F}{3})^q - F] - (F-1). \tag{21}$$

Obviously, Eq. (21) is different from Eq. (16). It leads to negative values for q$\in (0,1)$ and F smaller than 1. This apparent difference, at first glance, may look like a possible inconsistency in the nonextensive formalism, but let us look closer at these two different relative entropy expressions i.e., Eqs. (11) and (12) by trying to solve them within a perturbative approach. The reason for this is to ensure that all eigenvalues of σ are different than zero. From now on, we do not have to restrict ourselves to any particular interval of q as long as it is not equal to 1. In order to do this, let us rewrite σ as

$$\sigma = (1-\epsilon) \mid \Psi^-\rangle\langle\Psi^- \mid + \frac{\epsilon}{3}(1 - \mid \Psi^-\rangle\langle\Psi^- \mid). \tag{22}$$

This definition of σ corresponds to our earlier definition when we set ϵ equal to zero. If we recalculate Eqs. (11) and (12) now, we obtain

$$I_q(\rho_W \parallel \sigma) = \frac{1}{q-1}[(1-\epsilon)^q F^q + \epsilon^{1-q}(1-F)^q - 1)], \tag{23}$$

whereas Frank-Naudts version, we have

$$D_q(\rho_W \parallel \sigma) = \frac{1}{q-1}\ [F^q + 3^{1-q}(1-F)^q - (1-\epsilon)^{q-1}F - (\frac{\epsilon}{3})^{q-1}(1-F)] - (1-\epsilon)^{q-1}F - (\frac{\epsilon}{3})^{q-1}(1-F) + (1-\epsilon)^q + 3^{1-q}\epsilon^q. \tag{24}$$

Now let us consider the limit $\epsilon \to 0$ for these two distinct expressions of divergence assuming F to be between 0 and 1. Then, for q$\in (0,1)$, we obtain

$$I_q(\rho_W \parallel \sigma) = \frac{1}{1-q}(1-F^q). \tag{25}$$

and

$$D_q(\rho_W \parallel \sigma) = +\infty. \tag{26}$$

On the other hand, for q values greater than 1, we have

$$I_q(\rho_W \parallel \sigma) = +\infty. \tag{27}$$

and

$$D_q(\rho_W \parallel \sigma) = \frac{1}{q-1}\ [F^q + 3(\frac{1-F}{3})^q - F] - (F-1). \tag{28}$$

In order to understand the difference between Eqs. (11) and (12), we consider first the maximization of the functional

$$\Phi^{ordinary} = S_q - \alpha(\sum_i p_i - 1) - \beta(\sum_i p_i \varepsilon_i - U^{ordinary}), \tag{29}$$

where the superscript "ordinary" indicates that we are using ordinary expectation values. The equation above provides us the following solution

$$\widetilde{p_i}^{ordinary} = [1 + (1-q)\widetilde{S}_q^{ordinary}]^{1/(q-1)} \times [1 - \frac{q-1}{q}\beta\prime(\varepsilon_i - \widetilde{U}^{ordinary})]_+^{1/(q-1)}, \tag{30}$$

where tilda denotes that this particular expression is calculated in terms of the maximum entropy distribution $\widetilde{p_i}^{ordinary}$, and $\beta\prime$ is given by

$$\beta\prime = \frac{\beta}{\sum_i (\widetilde{p_i}^{ordinary})^q}. \tag{31}$$

If the normalized q-expectation value [27] is employed, the functional to be maximized will be of the form

$$\Phi^{normalized} = S_q - \alpha(\sum_i p_i - 1) - \beta(\frac{\sum_i p_i^q \varepsilon_i}{\sum_j p_j^q} - U^{normalized}), \tag{32}$$

which gives

$$\widetilde{p_i}^{normalized} = [1 + (1-q)\widetilde{S}_q^{normalized}]^{1/(1-q)} \times [1 - (1-q)\beta^*(\varepsilon_i - \widetilde{U}^{normalized})]_+^{1/(1-q)}, \tag{33}$$

where

$$\beta^* = \frac{\beta}{\sum_i (\widetilde{p_i}^{normalized})^q}. \tag{34}$$

If we now substitute $\widetilde{p_i}^{ordinary}$ given by Eq. (23) into Eq. (12), we obtain

$$D_q(p \parallel \widetilde{p_i}^{ordinary}) = \beta(F_q^{ordinary} - \widetilde{F}_q^{ordinary}), \tag{35}$$

i.e., the relative entropy of Bregman type is nothing but the difference of free energies when the ordinary expectation value is considered. This result has been derived also by T. D. Frank [28] by using a different technique than the one adopted in this paper. Similarly, if we now substitute $\widetilde{p_i}^{normalized}$ in Eq. (26) into Eq. (11), we get

$$I_q(p \parallel \widetilde{p_i}^{normalized}) = \beta^{**}(F_q^{normalized} - \widetilde{F}_q^{normalized}), \tag{36}$$

where $\beta^{**} = \frac{\sum_i (p_i)^q}{\sum_i (\widetilde{p_i}^{normalized})^q}\beta$. Eq. (29) shows us that the relative entropy of Csiszár type is nothing but the difference of free energies when the normalized q-expectation value is being used. Therefore, as far as their physical meanings are concerned, these two relative entropies are the same as Csiszár type, being connected with the normalized q-expectation values and Bregman type is depending on ordinary expectation values (for details, see Ref. [29]).

One can consider writing Eq. (28) in terms of normalized q-expectation values as is suggested by J. Naudts: This is tantamount to rewriting Eq. (22) by changing ordinary probability distributions to escort probability distributions and replacing q by 1/q. The escort probability distribution, which will be obtained after the maximization, must then be substituted into the following quantum divergence of Bregman type

$$D_q(\rho \parallel \sigma) = \frac{1}{(1/q)-1}\left[Tr(\rho^{1/q}) - Tr(\rho\sigma^{(1/q)-1})\right] - Tr(\rho\sigma^{(1/q)-1}) - Tr(\sigma^{1/q}). \tag{37}$$

If one now substitutes the new escort probability distribution which is obtained by the substitutions $p_i \rightarrow \frac{p_i^q}{\sum_j p_j^q} = P_i$ and $q \rightarrow 1/q$ into the equation above, we obtain the same free energy difference which has been obtained in Eq. (28) but this time with terms such as $\mathrm{F}_q^{normalized}$ and $\widetilde{F}_q^{normalized}$ i.e., normalized free energy expressions. This *prima facie* looks like the solution to our problem: We have obtained a relative entropy expresion in accordance with the third constraint, simply making some minor changes in the form of Eq. (12) and in the maximization procedure as explained above. This apparently simple solution has two flaws: First of all, in the last maximization procedure, we have used $\sum_i P_i = 1$. But, this simply means that we have chosen it as a constraint in our maximization. Now reminding ourselves that $\frac{p_i^q}{\sum_j p_j^q} = P_i$, we see that what we used as a constraint is nothing but an identity. If we choose to use this normalization as a constraint, then we must treat P_i as an independent variable. Once this had been assumed, the entropy written in terms of $\mathrm{P}_i's$ will be a new entropy which is different from Tsallis entropy. Secondly, $\mathrm{S}_q(P)$ occurs to be nonconcave in some intervals which has been shown by Abe [30] and Di Sisto et al. [31]. All these observations make it clear that we still do not have a plausible relative entropy definition of Bregman type.

III. RESULTS AND DISCUSSIONS

We have studied two definitions of relative entropy in current use in the nonextensive formalism. We have calculated the degree of purification of Werner state using quantum divergence as recently proposed by Jan Naudts and T. D. Frank and showed that it provides us a result different from the one obtained by S. Abe in Ref. [25] using the quantum divergence of Csiszàr type. This difference is traced to the fact that one of Bregman type is written in a way compatible with the first choice and the other is compatible with the third choice of constraint in the nonextensive formalism. The Bregman type gives rise to solutions for q values greater than 1 and F smaller than 1 whereas Csiszàr type is suitable for q values between 0 and 1. They differ in their qualitative behavior too because the Bregman type decreases as fidelity F decreases while the Csiszàr type increases as F decreases. This too is related to the choice of constraints. The problem of writing a relative entropy expression of Bregman type in the nonextensive formalism compatible with the third constraint is still an open question for further research.

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