Some remarks on Rényi relative entropy in a thermostatistical framework

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(Dated: December 28, 2021)

In ordinary Boltzmann-Gibbs thermostatistics, the relative entropy expression plays the role of generalized free energy, providing the difference between the off-equilibrium and equilibrium free energy terms associated with Boltzmann-Gibbs entropy. In this context, we studied whether this physical meaning can be given to Rényi relative entropy definition found in the literature from a generalized thermostatistical point of view. We find that this is possible only in the limit as $q$ approaches to 1. This shows that Rényi relative entropy has a physical (thermostatistical) meaning only when the system can already be explained by ordinary Boltzmann-Gibbs thermostatistics. Moreover, this can be taken as an indication of Rényi entropy being an equilibrium entropy since any relative entropy definition is a two-probability generalization of the associated entropy definition. We also note that this result is independent of the internal energy constraint employed. Finally, we comment on the lack of foundation of Rényi relative entropy as far as its minimization (which is equivalent to the maximization of Rényi entropy) is considered in order to obtain a stationary equilibrium distribution since Rényi relative entropy does not conform to Shore-Johnson axioms.

Keywords: Rényi relative entropy, entropy maximization, free energy, escort distribution, Shore-Johnson axioms

PACS numbers: PACS: 05.70.-a; 05.70.Ce; 05.70.Ln

I. INTRODUCTION

Recently there has been a growing interest in generalized entropies such as Tsallis [1], Rényi [2] and Sharma-Mittal [3] entropies in the context of a generalized thermostatistics. Although Rényi entropy has been introduced by A. Rényi as early as 1961, the applications of this form of entropy have been for example in the fields of quantum computation [4], information theory [5, 6] and chaotic one-dimensional maps [7]. Only recently, some authors have studied Rényi entropy in the framework of a generalized thermostatistics [8-12]. Lenzi et al. [8] and Bashkirov [11] for example showed that it results in a power-law equilibrium distribution by maximization whereas Parvan and Biró [12] concluded that Rényi entropy also satisfies zeroth law of thermodynamics. In this Letter, we will focus on the physical meaning of Rényi relative entropy (also called divergence or cross-entropy) in the framework of a generalized thermostatistics. Before proceeding further, it is important to assess the importance of relative entropy in entropy maximization related issues and in thermostatistics in general. For this purpose, let us write Boltzmann-Gibbs (BG) entropy which reads

$$S_{BG}(p) = -\sum_{i}^{W} p_i \ln p_i,$$

where $p_i$ is the probability of the system in the $i$th microstate, $W$ is the total number of the configurations of the system. Note that Boltzmann constant $k$ is set to unity throughout the paper. The corresponding relative entropy is called Kullback-Leibler entropy (K-L) [13] and it is given by

$$K[p||q] = \sum_{i} p_i \ln(p_i/q_i).$$

Note that it is a convex function of $p_i$, always non-negative and equal to zero if and only if $p = q$. The probabilities $q_i$’s are called prior or reference distributions. K-L entropy can be thought a generalization of BG entropy in the sense that both are equal to one another, apart from a multiplicative constant, when the prior distribution in relative entropy definition is known with certainty i.e., a probability of one is assigned to it. Therefore, it is always possible to obtain BG entropy as a particular case of corresponding relative entropy expression, so called K-L entropy. The converse is not true since K-L relative entropy is a two-probability distribution generalization of BG entropy. This situation can be compared to the case of Rényi and BG entropies: Rényi entropy is considered to be a generalization of BG entropy simply due to the fact that its parameter can be adjusted in such a way that it results in BG entropy as a particular case. Whenever the Rényi index $q$ becomes 1, we obtain BG entropy as a particular case. In this sense, any relative entropy definition associated with a particular entropy, be it Rényi or Tsallis entropies, is a generalization of that particular entropy in terms of probabilities whereas generalized entropies such as Rényi or Tsallis entropies are seen to be generalization in terms of some parameter $q$ although the nature of this parameter is not the same in these aforementioned cases. Second issue regarding the importance of the concept of rela-

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tive entropy is that ordinary BG entropy cannot be generalized to continuum rigorously just by changing summation to integration since it fails to be invariant under different parametrizations. Moreover, it will not be bounded neither from below nor above (see Ref.[14] and references therein). Contrary to these problems with ordinary BG entropy in its generalization to the continuum case, the relative entropy definition does not face any of these problems. Therefore, relative entropy is more general in its domain of applicability since it can be used in the continuum case unlike ordinary BG entropy. All of the remarks above can be summarized by the statement that the concept of relative entropy is a generalization of the corresponding entropy definition both in terms of probability distributions and continuum case. It is our aim in this paper to present some results related to the definition of Rényi relative entropy concerning its physical meaning and relation to internal energy constraints. But since Rényi relative entropy is understood to be a generalization of Rényi entropy, what can be said about Rényi relative entropy has important bearings on Rényi entropy itself. In addition to these important features of relative entropy in a thermostatistical framework, it is also an important measure of complexity whose uses range from the numerical analysis of protein sequences [15], pricing models in the market [16], to medical decision making [17]. The outline of the Letter is as follows: In the next Section, we revisit the physical meaning of the ordinary relative entropy in the case of BG entropy. We then study Rényi relative entropy in a thermostatistical framework in Section III. Section IV will be devoted to the study of the axiomatic foundation of Rényi relative entropy. The conclusions will be discussed in Section V.

II. PHYSICAL MEANING OF KULLBACK-LEIBLER RELATIVE ENTROPY

In order to study the physical meaning of any relative entropy in a thermostatistical framework, one has first to obtain the equilibrium distribution associated with the entropy of that particular thermostatistics. In this Section, we will maximize BG entropy subject to some constraints following the well known recipe of entropy maximization. Let us assume that the internal energy function is given by $U = \sum_i \varepsilon_i p_i$, where $\varepsilon_i$ denotes the energy of the $i$th microstate. In order to get the equilibrium distribution associated with BG entropy, we maximize the following functional

$$\Phi(p) = -\sum_i p_i \ln p_i - \alpha \sum_i p_i - \beta \sum_i \varepsilon_i p_i,$$

where $\alpha$ and $\beta$ are Lagrange multipliers related to normalization and internal energy constraints respectively.

Equating the derivative of the functional to zero, we obtain

$$\frac{\delta \Phi(p)}{\delta p_i} = -\ln p_i - 1 - \alpha - \beta \varepsilon_i = 0. \quad (4)$$

Tilde denotes the equilibrium distribution obtained by the maximization of BG entropy. By multiplying Eq. (4) by $\tilde{p}_i$ and summing over $i$, using the normalization and internal energy constraints, we have

$$\alpha + 1 = \tilde{S}_{BG} - \beta \tilde{U}. \quad (5)$$

Substitution of Eq. (5) into Eq. (4) results in the following equilibrium distribution

$$\tilde{p}_i = e^{-\tilde{S}_{BG}/\beta} e^{\tilde{U}} e^{-\beta \varepsilon_i}. \quad (6)$$

If we now use the equilibrium distribution $\tilde{p}$ as the reference distribution in K-L entropy, we can write

$$K[p\|\tilde{p}] = \sum_i p_i \ln(p_i/\tilde{p}_i). \quad (7)$$

The equation above can be rewritten as

$$K[p\|\tilde{p}] = -\tilde{S}_{BG} - \sum_i p_i \ln \tilde{p}_i. \quad (8)$$

We then insert the equilibrium distribution given by Eq. (6) in the equation above to find

$$K[p\|\tilde{p}] = -\tilde{S}_{BG} - \sum_i p_i (-\tilde{S}_{BG} + \tilde{U}) - \beta \varepsilon_i. \quad (9)$$

Carrying out the summation, we have

$$K[p\|\tilde{p}] = -\tilde{S}_{BG} + \tilde{S}_{BG} - \beta \tilde{U} + \tilde{U}, \quad (10)$$

which can be cast into the form

$$K[p\|\tilde{p}] = \beta(F_{BG} - \tilde{F}_{BG}). \quad (11)$$

The free energy term is given as usual by $F = U - S_{BG}/\beta$. The result above shows us that the physical meaning of the K-L entropy is nothing but the difference of the off-equilibrium and equilibrium free energies when the reference distribution is taken to be the equilibrium distribution given by Eq. (6) above. This result can be used, for example, to study equilibrium fluctuations or non-equilibrium relaxation of polymer chains [18].
III. RÉNYI RELATIVE ENTROPY AS A GENERALIZED FREE ENERGY

After studying the physical meaning of K-L entropy in the previous Section, we are now ready to study the meaning of Rényi relative entropy in generalized thermodynamical framework. In order to do this, we begin by writing Rényi entropy \[2\]

\[ S_R(p) = \frac{1}{1-q} \ln \left( \sum_i p_i^q \right), \quad (12) \]

where the parameter \( q \) is an arbitrary real number. Rényi entropy is equal to or greater than zero for all values of the parameter \( q \) and concave for \( q \leq 1 \). It reduces to BG entropy given by Eq. (1) as the parameter \( q \) approaches 1. Using internal energy constraint in terms of escort probabilities i.e., \( U_q = \frac{\sum_i \varepsilon_i p_i^q}{\sum_i p_i^q} \), the functional to be maximized reads

\[ \Phi_R(p) = \frac{1}{1-q} \ln \left( \sum_i p_i^q \right) - \alpha \sum_i p_i - \beta \frac{1}{\sum_i p_i^q} \sum_i \varepsilon_i p_i^q. \quad (13) \]

We take the derivative of this functional and equate it to zero in order to obtain the following

\[ \frac{\delta \Phi_R(p)}{\delta p_i} = \frac{q}{1-q} \frac{\tilde{p}_i^{q-1}}{\sum_j \tilde{p}_j^q} - \beta q^{q-1} (\varepsilon_i - \bar{U}_q) = 0, \quad (14) \]

where \( \beta^* \) is given by

\[ \beta^* = \frac{\beta}{\sum_j \tilde{p}_j^q}. \quad (15) \]

Multiplying the equation above by \( \tilde{p}_i \) and summing over the index \( i \), we find

\[ \alpha = \frac{q}{1-q}. \quad (16) \]

Note that tilde denotes that the distribution is calculated at equilibrium. Substituting this explicit expression of \( \alpha \) into Eq. (14), we calculate the explicit form of equilibrium distribution . It reads

\[ \tilde{p}_i = \left( \frac{1}{e^{(1-q)\bar{S}_R}} - (1-q)\beta^*(\varepsilon_i - \bar{U}_q) \right)^{1/(1-q)}. \quad (17) \]

The Rényi relative entropy \[19\] reads

\[ I_q[p||r] = \frac{1}{q-1} \ln \left( \sum_i p_i^q r_i^{1-q} \right). \quad (18) \]

This definition of Rényi relative entropy too is always non-negative and equal to zero if and only if \( p = r \). It also reduces to K-L entropy as the parameter \( q \) approaches 1. We then substitute equilibrium distribution in Eq. (17) into the relative entropy definition above and obtain

\[ I_q[p||\bar{p}] = \frac{1}{q-1} \ln \left( \sum_i p_i^q \left( \frac{1}{e^{(1-q)\bar{S}_R}} - (1-q)\beta^*(\varepsilon_i - \bar{U}_q) \right) \right). \quad (19) \]

Having summed up over indices, we obtain

\[ I_q[p||\bar{p}] = \frac{1}{q-1} \ln(e^{(1-q)(\bar{S}_R - \bar{S}_R)} - (1-q)\beta^{**}(U_q - \bar{U}_q)), \quad (20) \]

where \( \beta^{**} \) is given by

\[ \beta^{**} = \frac{\beta}{\sum_j p_j^q} \sum_i p_i^q. \quad (21) \]

Inspection of Eq. (20) shows that one cannot cast it into the form of free energy differences associated with Rényi-related quantities due to the logarithmic term involved. Indeed, one needs to apply Taylor expansion two times, first to the exponential term in the parentheses and second to the logarithmic term itself. Having made these two Taylor series expansions about \( q = 1 \), we finally arrive a familiar result i.e.,

\[ I_q[p||\bar{p}] = \beta(F_{BG} - \bar{F}_{BG}), \quad (22) \]

where free energy expressions are exactly the same as in the BG case. This result is trivial and equal to the expression obtained in Section II by using BG entropy and K-L entropy. It should be noted that the first Taylor expansion turned the Rényi entropy into BG entropy while second Taylor expansion turned the Lagrange multiplier and internal energy functions into their corresponding BG values.

It is important to underline one crucial point: we have maximized Rényi entropy with escort distribution and used this equilibrium distribution as the reference distribution for the associated relative entropy expression. However, if we try to maximize it with ordinary constraint, then we obtain

\[ \tilde{p}_i = [(1 - \beta \frac{q-1}{q} (\varepsilon_i - \bar{U}_q)) \sum_j \tilde{p}_j^{q/(1-q)}]. \quad (23) \]

for the equilibrium distribution. It is obvious that the substitution of Eq. (23) into relative entropy expression given by Eq. (18) does not yield to a result which can be written as difference of free energies for all \( q \) values. Again, the relative entropy will be a generalized free energy only in the limit as \( q \) approaches 1. This shows that the choice of internal energy constraint does not matter at all in assessing the physical meaning of Rényi relative entropy.
IV. AXIOMATIC FOUNDATION OF RÉNYI RELATIVE ENTROPY

The stationary equilibrium distribution associated with a particular entropy expression can be found either by the maximization of that entropy or the minimization of the corresponding relative entropy. In this sense, it is expected both of these methods to be consistent and well-founded in terms of axioms. Shore and Johnson considered the axioms, which must be satisfied by any relative entropy expression if they were expected to lead to minimum relative entropy for the stationary equilibrium distribution in a consistent manner [20, 21]. These axioms are given by

1. Axiom of Uniqueness: If the same problem is solved twice, then the same answer is expected to result both times.

2. Axiom of Invariance: The same answer is expected when the same problem is solved in two different coordinate systems, in which the posteriors in the two systems should be related by the coordinate transformation.

3. Axiom of System Independence: It should not matter whether one accounts for independent information about independent systems separately in terms of their marginal distributions or in terms of the joint distribution.

4. Axiom of Subset Independence: It should not matter whether one treats independent subsets of the states of the systems in terms of their separate conditional distributions or in terms of the joint distribution.

5. Axiom of Expansibility: In the absence of new information, the prior should not be changed.

These authors were able to show that the satisfaction of all these axioms resulted in a relative entropy expression consistent with the principle of minimum relative entropy and could be summarized in one simple expression: according to Shore and Johnson, any relative entropy $J[p||r]$ with the prior $r_i$ and posterior $p_i$ which satisfies five very general axioms, must be of the form

$$J[p||r] = \sum_i p_i h(p_i/r_i),$$

(24)

for some function $h(x)$. Ordinary relative entropy i.e., K-L entropy is in accordance with Shore-Johnson theorem since the function $h(x)$ can be identified as the natural logarithm. In the case of Rényi relative entropy given by Eq. (18), we see that it cannot be cast into a form which will conform to the Shore-Johnson theorem for any function $h(x)$. In other words, there is no axiomatic basis for the use of Rényi relative entropy in order to get the stationary equilibrium distribution for a possible generalized thermostatistics.

V. CONCLUSIONS

The relative entropy acts as a generalized free energy in the ordinary thermostatistical framework when one makes use of the associated equilibrium distribution as the reference distribution. In this Letter, we investigated whether Rényi relative entropy can play the role of a generalized free energy in a thermostatistical framework. We found that this is possible only in the limit as $q$ approaches to 1. This shows that Rényi relative entropy has a thermostatistical meaning only when the system is in a state of ordinary BG thermostatistics. This can be taken as an indication of Rényi entropy being an equilibrium entropy and nothing but an approximation to ordinary BG thermostatistics since any relative entropy definition is a two-probability generalization of the associated entropy definition. The choice of internal energy constraint too does not solve the problem. Still, relative entropy acts as a generalized free energy only in the $q=1$ limit. This is different than the case of BG or Tsallis entropy [21]. In Tsallis case in particular, one does not need to make any approximation, which in turn makes the physical interpretation valid for all positive $q$ values. This is reminiscent of the fact that Rényi entropy provides the same answer at the microcanonical structure as BG entropy, yielding $lnW$ [22]. As Rényi entropy yields the same result as BG entropy in the microcanonical case, so does Rényi relative entropy in its connection to free energies. In other words, it is redundant to use Rényi entropy in the microcanonical case and it is so to use Rényi relative entropies in calculating nonequilibrium fluctuations of polymer chains since we already have K-L entropy for this purpose [18]. These results regarding the physical meaning of Rényi relative entropy are similar to the results derived from Lesche stability condition [23] for Rényi entropy since both considers deformation of probabilities and concludes Rényi entropy makes sense only in the limit when $q$ approaches 1 in which case it becomes BG entropy (corresponding relative entropy becomes K-L entropy). Lastly, it can be noted that the results presented in this paper are also supported by the original methodology of orthotheses devised by Boltzmann when applied to Rényi entropy since it leads one to deduce that Rényi entropy is an equilibrium entropy [24]. It is interesting to note that this result has also been reached independently in Ref. [25] by using a different method than the method of orthotheses employed in Ref. [24] thereby making this view even stronger. Our approach to this issue explains one more difficulty arising from the comparison of the works of Refs. [24] and [25] since in the former escort distribution has been employed whereas ordinary constraint has been used in the latter. In our view, it is not surprising that the same conclusion has been reached concerning Rényi entropy being an equilibrium entropy since associated relative entropy possesses a physical meaning in both cases only when the parameter $q$ approaches 1, thereby making the difference in employed constraints redundant. Apart from the
verification of this result, it can be noted that the novelty here is the understanding of this entropy to be an approximation to the ordinary BG entropy in the thermostatistical framework in a generalized setting of the definition of corresponding relative entropy. Lastly, we have shown that Rényi relative entropy does not have a sound axiomatic foundation since it does not conform to Shore-Johnson axioms. Therefore, any attempt to minimize Rényi relative entropy in order to obtain an associated stationary equilibrium distribution in the context of generalized thermostatistics fails to be consistent.

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