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# The Physical Meaning of the Rényi Relative Entropy

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**Abstract:** The Boltzmann-Gibbs relative entropy provides the difference between the off-equilibrium and equilibrium free energy terms associated with Boltzmann-Gibbs entropy. In this work, we studied whether this physical meaning can be given to Rényi relative entropy definition. We find that this is possible only in the limit as $q$ approaches to 1. This shows that Rényi relative entropy has a physical meaning only when the system can already be explained by ordinary Boltzmann-Gibbs entropy. We also note that this result is independent of the internal energy constraint employed.

# Rényi Göreceli Entropisinin Fiziksel Anlamı

**Anahtar Kelimeler**
Rényi göreceli entropisi,
Serbest enerji,
Entropi maksimizasyonu

**Özet:** Boltzmann-Gibbs göreceli entropisi, Boltzmann-Gibbs entropisine ilişkin denge dışı ve denge durumları arasındaki serbest enerji farkını vermektedir. Bu çalışmada, böyle bir fiziksel anlamın Rényi göreceli entropi tanımına verilip verilemeyeceğini araştırdık. Bu türden bir fiziksel anlamın sadece $q$ değeri 1'e yaklaştığında mümkün olduğunu bulduk. Bu sonuç göstermektedir ki, Rényi göreceli entropisi sadece sistem zaten Boltzmann-Gibbs entropisi tarafından açıklanabildiğinde bir fiziksel anlama sahip olmaktadır. Ayrıca bulunan bu sonucun kullanılan iç enerji kısıtından da bağımsız olduğu gösterilmiştir.

## 1. Introduction

Although Rényi entropy has been introduced by A. Rényi as early as 1961 [1], only recently some authors have studied Rényi entropy in the framework of a generalized thermostatistics [2, 3]. Lenzi et al. [2] and Bashkirov [3] for example showed that it results in a power-law equilibrium distribution by maximization. In this work, we will focus on the physical meaning of Rényi relative entropy (also called divergence or cross-entropy) in the framework of a generalized thermostatistics. Rényi relative entropy has been used to study Hadamard channels [4], squashed entanglement [5], conformal field theories [6], entropic uncertainty relations [7] and quantum coherence [8]. 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

$$S_{BG}(p) = -\sum_{i}^{W} p_i \ln p_i, \qquad (1)$$

where $\mathrm{p_i}$ is the probability of the system in the ith 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) [9] and it is given by

$$K[p\|q] \equiv \sum_{i} p_i \ln(p_i/q_i). \qquad (2)$$

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 as 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

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$q$ although the nature of this parameter is not the same in these aforementioned cases. Second issue regarding the importance of the concept of relative 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.[10] 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. The outline of the paper 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 3. The discussion and conclusion will be discussed in Section 4.

## 2. 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 ith microstate. In order to get the equilibrium distribution associated with BG entropy, we maximize the following functional

$$\Phi(p) = -\sum_i^W p_i \ln p_i - \alpha \sum_i^W p_i - \beta \sum_i^W \varepsilon_i p_i, \tag{3}$$

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

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

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

$$\alpha + 1 = \widetilde{S}_{BG} - \beta \widetilde{U}. \tag{5}$$

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

$$\widetilde{p}_i = e^{-\widetilde{S}_{BG}} e^{\beta \widetilde{U}} e^{-\beta \varepsilon_i}. \tag{6}$$

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

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

The equation above can be rewritten as

$$K[p \| \widetilde{p}] = -S_{BG} - \sum_i p_i \ln \widetilde{p}_i. \tag{8}$$

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

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

Carrying out the summation, we have

$$K[p \| \widetilde{p}] = -S_{BG} + \widetilde{S}_{BG} - \beta \widetilde{U} + \beta U, \tag{10}$$

which can be cast into the form

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

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 [11].

## 3. 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 thermostatistical framework. In order to do this, we begin by writing Rényi entropy [1]

$$S_R(p) = \frac{1}{1-q} \ln(\sum_i p_i^q), \tag{12}$$

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., $U_q = \frac{\sum_i \varepsilon_i p_i^q}{\sum_j p_j^q}$, the functional to be maximized reads

$$\Phi_R(p) = \frac{1}{1-q} \ln(\sum_i^W p_i^q) - \alpha \sum_i^W p_i - \beta \frac{\sum_i^W \varepsilon_i p_i^q}{\sum_i^W p_j^q}. \tag{13}$$

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

$$\frac{\delta \Phi_R(p)}{\delta p_i} = \frac{q}{1-q} \frac{\widetilde{p}_i^{q-1}}{\sum_j \widetilde{p}_j^q} - \alpha - \beta^* q \widetilde{p}^{q-1} (\varepsilon_i - \widetilde{U}_q) = 0, \tag{14}$$

where $\beta^*$ is given by

$$\beta^* = \frac{\beta}{\sum_j \widetilde{p}_j^q}. \tag{15}$$

Multiplying the equation above by $\widetilde{p}_i$ and summing over the index i, we find

$$\alpha = \frac{q}{1-q}. \tag{16}$$

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

$$\widetilde{p}_i = \left(\frac{1}{e^{(1-q)\widetilde{S}_R}} - (1-q)\beta^* (\varepsilon_i - \widetilde{U}_q)\right)^{1/(1-q)}. \tag{17}$$

The Rényi relative entropy [19] reads

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

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

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

Having summed up over indices, we obtain

$$I_q[p \| \widetilde{p}] = \frac{1}{q-1} \ln\left(e^{(1-q)(S_R - \widetilde{S}_R)} - (1-q)\beta^{**} (U_q - \widetilde{U}_q)\right), \tag{20}$$

where $\beta^{**}$ is given by

$$\beta^{**} = \frac{\beta}{\sum_j \widetilde{p}_j^q} \sum_i p_i^q. \tag{21}$$

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.,

$$I_q[p \| \widetilde{p}] = \beta (F_{BG} - \widetilde{F}_{BG}), \tag{22}$$

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 2 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

$$\widetilde{p}_i = \left[\left(1 - \beta \frac{q-1}{q} (\varepsilon_i - \widetilde{U}_q)\right) \sum_j \widetilde{p}_j^q\right]^{1/(q-1)}. \tag{23}$$

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.

## 4. Discussion and Conclusion

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. In other words, it is redundant to use Rényi relative entropy in calculating nonequilibrium fluctuations of polymer chains, since we already have K-L entropy for this purpose [11]. It can also be noted that the results presented in this paper are also supported by the original methodology of orthodes devised by Boltzmann when applied to Rényi entropy since it leads one to deduce that Rényi entropy is an equilibrium entropy [13]. It is interesting to note that this result has also been reached independently in Ref. [14] by using a different method than the method of orthodes employed in Ref. [13] thereby making this view even stronger. Our approach to this issue explains one more difficulty arising from the comparison of the works of Refs. [13] and [14], 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, Misra *et al.* recently showed that the relation between the free energy difference and the Rényi relative entropy can be restored at the expense of introducing an *ad-hoc* term $\Delta_{\alpha}^{'}$ (see Eq. (7) in [15]). This result is consistent with ours, since we have shown that the free energy difference cannot be equal to the Rényi relative entropy *per se*. However, Misra *et al.* does not notice that they break a fundamental connection with the statistical mechanics by doing so: these authors always use the internal energy definition as $U_q = \frac{\sum_i \varepsilon_i p_i^q}{\sum_j p_j^q}$, which yields $U_q = \frac{\sum_i \varepsilon_i p_i}{\sum_j p_j}$ in the limit $q \to 1$. In other words, their maximizing functional (i.e. just before the maximization is carried out) includes an internal energy definition $U_q = \frac{\sum_i \varepsilon_i p_i}{\sum_j p_j}$ which does not correspond to the ordinary functional of the Boltzmann-Gibbs case, since the normalization is not assumed in this functional but more so right after the maximization process. Therefore, these authors recover the link between Boltzmann-Gibbs and the Rényi entropy by assuming $\frac{\sum_i \varepsilon_i p_i}{\sum_j p_j} = \sum_i \varepsilon_i p_i$ even before the normalization is carried out. This of course does not make any sense for a consistent thermodynamics. Our result, however, is independent of the internal energy constraints used.

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