Information measures based on Tsallis' entropy and geometric considerations for thermodynamic systems

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Abstract

An analysis of the thermodynamic behavior of quantum systems can be performed from a geometrical perspective investigating the structure of the state space. We have developed such an analysis for nonextensive thermostatistical frameworks, making use of the q-divergence derived from Tsallis' entropy. Generalized expressions for operator variance and covariance are considered, in terms of which the fundamental tensor is given.
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1. Introduction

The geometrization of thermodynamics and statistical mechanics has been the subject of many studies during the last few decades. Among the collection of works related with this topic, different approaches have been followed. For instance, Weinhold [1] considered the thermodynamic surface given by the fundamental relation $U = U(\{X_i\})$ in the $(r + 1)$-dimensional Gibbs space (with coordinates labelled by $U, X_1, \ldots, X_r$), and obtained the components of the metric tensor of that space as the second derivatives of the internal energy U with respect to each pair of the r extensive parameters X_i. Ruppeiner [2] focuses attention on fluctuations of the thermodynamic magnitudes and obtains the metric tensor via second moments of the fluctuations. The two ensuing metrics have been proven by Mrugała to be equivalent [3]. Another statistical path for reaching a Riemannian metric [4] in the space of thermodynamic parameters is that originated in the works by Rao [5] and Amari (see, for instance, [6]) in the field of statistical mathematics, and also by Ingarden [7], Janyszek [8], and other authors in the field of thermodynamics and statistical mechanics. The concomitant information-theoretic approach is based on the concept of relative entropy and given in terms of the Boltzmann–Gibbs–Shannon entropy. The ensuing formalism has been applied to a number of model systems, from the ideal and van der Waals gases to the Ising and other magnetic models. In these applications it has been seen that the scalar curvature R of the space can represent a measure of the thermodynamic stability of the system, and a

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useful quantity to characterize phase transitions (typically, for noninteracting models one obtains $R = 0$, i.e. a flat geometry, while R diverges at the critical point for interacting systems). There are some recent efforts in the field of information geometry related with the generalized, nonextensive formulation of statistical mechanics [9]. Among these studies one finds the analysis by Abe [10] of the geometry of escort distributions, and the contributions by Amari, Nagaoka and coworkers ([6], among others) in connection with the geometrical structure in the manifold of probability distributions. A new geometrical approach to thermo-statistical mechanics is introduced in Ref. [11], where the relevance of the approach within the contexts of nonextensive statistical thermodynamics is analyzed, showing that Riemannian geometry concepts yield a powerful tool. More recently, Naudts [12] studies escort density operators and generalized Fisher information measures.

Here, our aim is to discuss in some detail the generalization of the geometrical approach to statistical physics. For that purpose we appeal to a generalized form for the entropy, as given by Tsallis [9]. The q-entropy is employed in order to define an information measure from which we can derive the metrical structure of the parameters' space. The generalization of the definitions of variance and covariance for quantum operators in the context of the so-called OLM version [13] of nonextensive statistical mechanics is developed. The metric is finally expressed in terms of generalized fluctuations.

2. OLM density operator

For a given quantum mechanical system, the density operator that maximizes Tsallis' nonextensive q-entropy [9] $S_q \equiv k_B(1 - \text{Tr}\,\hat{\rho}^q)/(q-1)$ (with $q \in \mathbb{R}^+$ and $k_B \equiv 1$) is written, within the optimized Lagrange multipliers' (OLM) formalism [13], as $\hat{\rho} = \bar{Z}_q^{-1} e_q(-\sum_{i=1}^r \lambda_i(\hat{F}_i - m_i))$. Here, the generalized expectation values of r quantum operators $\{\hat{F}_1, \ldots, \hat{F}_r\}$ are considered to be known as prior information; they are given by $m_i = \langle \hat{F}_i \rangle_q = \text{Tr}(\hat{\rho}^q \hat{F}_i)/\text{Tr}\,\hat{\rho}^q$, $i = 1, \ldots, r$. The parameters $\{\lambda_1, \ldots, \lambda_r\}$ refer to the set of Lagrange multipliers that fit those restrictions in the procedure of constrained extremization of S_q when one is working *within the OLM formalism*, i.e. the restrictions are rewritten as $\text{Tr}\,\hat{\rho}^q(\hat{F}_i - m_i) = 0$. It has been established [14] that $\{\lambda_i\}$ correspond to the *physical* intensive parameters. In this OLM framework, the pseudo-partition function $\bar{Z}_q \equiv \text{Tr}\,e_q(-\sum \lambda_i(\hat{F}_i - m_i))$ is such that the density operator is normalized, i.e. $\text{Tr}\,\hat{\rho} = 1$. Notice that the Lagrange multiplier associated with the normalization condition is not written explicitly in the equilibrium density matrix, instead we chose to introduce the q-partition function $\bar{Z}_q$ in the expression for $\hat{\rho}$. In all these expressions, $e_q(x)$ stands for the q-exponential function: $e_q(x) \equiv [1 + (1-q)x]_+^{1/(1-q)}$, with $[X]_+ = \max\{0, X\}$. The extensive limit corresponds to the situation $q \to 1$, and then $q - 1$ is a measure of the degree of entropy nonextensivity.

3. Generalized variances

We begin by providing a natural q-generalization of the variance of an operator and of the covariance between two operators. For this purpose we address the relation between fluctuation and response in nonextensive settings [15]. We need then to compute the derivative of each mean value with respect to every Lagrange multiplier, which poses a rather intricate problem. A linear system of r coupled equations is to be faced for each λ. This system can be solved and, after some manipulations, the following result is reached:

$$\frac{\partial m_i}{\partial \lambda_j} = -q\,\bar{Z}_q^{q-1}\left(1 - q\bar{Z}_q^{q-1}\sum_{l=1}^r \lambda_l \langle \hat{\rho}^{q-1}\delta_q\hat{F}_l \rangle_q\right)^{-1}\left[\langle \hat{\rho}^{q-1}\,\delta_q\hat{F}_i\,\delta_q\hat{F}_j \rangle_q - q\bar{Z}_q^{q-1}\right.$$
$$\left.\times\left(\langle \hat{\rho}^{q-1}\,\delta_q\hat{F}_i\,\delta_q\hat{F}_j \rangle_q \sum_{l=1}^r \lambda_l \langle \hat{\rho}^{q-1}\delta_q\hat{F}_l \rangle_q - \langle \hat{\rho}^{q-1}\,\delta_q\hat{F}_i \rangle_q \sum_{l=1}^r \lambda_l \langle \hat{\rho}^{q-1}\,\delta_q\hat{F}_j\,\delta_q\hat{F}_l \rangle_q\right)\right]$$

where $\delta_q\hat{F}_i \equiv \hat{F}_i - m_i$ are the generalized deviation operators, and $\hat{\rho}$ is the OLM density matrix. For the sake of simplicity, we have considered here a set of r *commuting* operators. Let us stress that the derivative with

respect to a given λ_j is done keeping all other $\lambda_{j'}$ ($j' \neq j$) fixed. After writing down the above equation it seems advantageous for us to advance the following definitions for q-generalized deviations, covariances, and squared variances or dispersions, respectively:

$$(\delta_q F_i) \equiv \langle \hat{\rho}^{q-1} \delta_q \hat{F}_i \rangle_q, \tag{1}$$

$$C_q(\hat{F}_i, \hat{F}_j) = \langle \hat{\rho}^{q-1} \delta_q \hat{F}_i \delta_q \hat{F}_j \rangle_q \quad \text{and} \quad (\Delta_q F_i)^2 \equiv C_q(\hat{F}_i, \hat{F}_i). \tag{2}$$

These can be interpreted as modified first and second moments of the corresponding operators. For the sake of completeness, we also define the generalized correlation coefficient to be $\mathscr{C}_q(\hat{F}_i, \hat{F}_j) \equiv C_q(\hat{F}_i, \hat{F}_j)/(\Delta_q F_i \Delta_q F_j)$, that equals 1 whenever $i = j$ for *arbitrary* values of q. Regarding the first definition, Eq. (1), the generalized expectation value in the r.h.s. will *not* be equal to zero in general—notice that, as it is given here, it is not the q-mean value of the q-deviation operator−; however $\lim_{q \to 1}(\delta_q F_i) = 0$. The expressions in Eq. (2) for the second moments differ from those given in Ref. [16] in a factor $\hat{\rho}^{q-1}$ inside the q-expectation values, that can be recast as $\bar{Z}_q^{1-q}[1 - (1 - q) \sum \lambda_l \delta_q \hat{F}_l]_+^{-1}$ (a similar factor has also been found in the computation of the generalized specific heat for an ideal Fermi gas [17]). Typical of the nonextensive statistical formalism is the emergence of *correlations* among different observables—induced by the nature of the q-statistics—with one quantity depending on *all* other ones (this has also been discussed for the occupation numbers in fermionic systems [17]).Nevertheless, one always finds the correct uncorrelated limit for $q \to 1$. Due to the presence of the density-dependent factor in Eq. (2), the evaluation of the q-variances and q-covariances involves not only quadratic terms with $\hat{F}_i \hat{F}_j$ (as required in the extensive limit) but the computation of $(r + 1)(r + 2)/2$ traces, apart from $\text{Tr} \, \hat{\rho}^q$, for a complete description of the correlations for a given problem. Indeed we can write

$$(\Delta_q F_i)^2 = \langle \hat{\rho}^{q-1} \hat{F}_i^2 \rangle_q - 2m_i \langle \hat{\rho}^{q-1} \hat{F}_i \rangle_q + m_i^2 \langle \hat{\rho}^{q-1} \rangle_q, \tag{3}$$

$$C_q(\hat{F}_i, \hat{F}_j) = \langle \hat{\rho}^{q-1} \hat{F}_i \hat{F}_j \rangle_q - m_i \langle \hat{\rho}^{q-1} \hat{F}_j \rangle_q - m_j \langle \hat{\rho}^{q-1} \hat{F}_i \rangle_q + m_i m_j \langle \hat{\rho}^{q-1} \rangle_q. \tag{4}$$

A bit of additional algebra finally yields one of our important results, namely,

$$\left. \frac{\partial m_i}{\partial \lambda_j} \right|_{\{\lambda_{j' \neq j}\}} = -q \bar{Z}_q^{q-1} \left(C_q(\hat{F}_i, \hat{F}_j) + \frac{q \bar{Z}_q^{q-1} (\delta_q F_i) \sum \lambda_l C_q(\hat{F}_j, \hat{F}_l)}{1 - q \bar{Z}_q^{q-1} \sum \lambda_l (\delta_q F_l)} \right). \tag{5}$$

4. The fundamental tensor

The fundamental tensor of the space of parameters, a key ingredient in the geometric approach to thermostatistics, can be interpreted in terms of thermodynamic fluctuations. Indeed, in the case of classical systems or commuting operators, the metric tensor derived within a standard treatment is equal to the covariance or second moment: $g_{ij}^{(1)} = \langle (\hat{F}_i - \langle \hat{F}_i \rangle)(\hat{F}_j - \langle \hat{F}_j \rangle) \rangle = C_1(\hat{F}_i, \hat{F}_j)$. For noncommuting operators, an integral expression for the covariances has been introduced [18], based on the connection with the metric tensor. We present in this section the formalism leading to analogous results within generalized statistical contexts.

A quantum state described by the density operator $\hat{\rho}(\lambda_1, \ldots, \lambda_r)$ can be represented in the r-dimensional space of parameters. The *information distance* between two normalized states can be given in terms of the symmetrized form of the relative entropy, which in a nonextensive context has been defined as [19] $K_q(\hat{\rho} \| \hat{\sigma}) = \text{Tr} \, \hat{\rho}^q (\ln_q \hat{\rho} - \ln_q \hat{\sigma})$, where $\ln_q(x)$ stands for the inverse function of $e_q(x)$. We compute then the symmetric information measure for a pair of density matrices, $\hat{\rho}(\{\lambda\})$ and $\hat{\rho}(\{\lambda + \partial \lambda\})$, and make an expansion around $\{\lambda\}$. The first nonvanishing contribution is the second order one, $\sum \partial \lambda_i \partial \lambda_j \, q \, \text{Tr}(\hat{\rho}^q) \langle \hat{\rho}^{-q-1} \partial_j \hat{\rho} \, \partial_i \hat{\rho} \rangle_q$ (where $\partial_i X \equiv \partial X/\partial \lambda_i$), which finally gives us the q-metric tensor as

$$g_{ij}^{(q)} = q \, \bar{Z}_q^{q-1} [C_q(\hat{F}_i, \hat{F}_j) - \partial_i \ln \bar{Z}_q \, (\delta_q F_j) - \partial_j \ln \bar{Z}_q \, (\delta_q F_i)$$
$$+ \partial_i \ln \bar{Z}_q \, \partial_j \ln \bar{Z}_q (\langle \hat{\rho}^{q-1} \rangle_q - \bar{Z}_q^{1-q})]. \tag{6}$$

Given in this shape, the evaluation of the generalized metric tensor for a given system requires knowledge of the pseudo-partition function and its logarithmic derivatives with respect to the Lagrange parameters, and also the generalized fluctuations.

Summing up, we have discussed appropriate definitions of q-variance and q-covariance for quantum operators in a generalized thermostatistical framework characterized by the nonextensivity index q, along the paths of Ref. [15]. Previous related literature is based on the generalized definitions given in Ref. [16]. Then, we have found the fundamental tensor of the space of thermodynamic parameters within a nonextensive statistical framework, in terms of quantum fluctuations. Application of these ideas to certain physical systems may contribute to characterize its thermodynamic behavior. In this sense we expect that the geometric analysis of the model, when performed in a generalized context with a value of q different from 1, may exhibit in a more clear way the critical regions.

Acknowledgments

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