Generalized statistical complexity and
Fisher-Rényi entropy product in the $H$-atom

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Abstract

By using the Rényi entropy, and following the same scheme that in the Fisher-Rényi entropy product case, a generalized statistical complexity is defined. Several properties of it, including inequalities and lower and upper bounds are derived. The hydrogen atom is used as a test system where to quantify these two different statistical magnitudes, the Fisher-Rényi entropy product and the generalized statistical complexity. For each level of energy, both indicators take their minimum values on the orbitals that correspond to the highest orbital angular momentum. Hence, in the same way as happens with the Fisher-Shannon and the statistical complexity, these generalized Rényi-like statistical magnitudes break the energy degeneration in the H-atom.

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1. INTRODUCTION

Nowadays the study of statistical magnitudes in quantum systems has a role of growing importance. So, information entropies and statistical complexities have been calculated on different atomic systems [1, 2]. In particular, the $H$-atom is a natural test system where to quantify all this kind of magnitudes [3, 4, 5, 6, 7]. This system displays a remarkable property when Fisher-Shannon information [8, 9, 10] and the so called LMC complexity [11, 12] are computed on it. Namely, for each energy level, the minimum values of those statistical measures are taken on the wave functions with the highest orbital angular momentum, those orbitals that correspond to the Bohr-like orbits in the pre-quantum image [7].

Shannon information [13] plays an important role in both entropic products, the Fisher-Shannon information and the LMC statistical complexity. Different generalizations of the Shannon information dependent on a parameter $\alpha$ can be found in the literature [14, 15]. Implementing these $\alpha$-entropies in both entropic products, different families of statistical indicators can be generated [16]. In particular, if Rényi entropies are taken in exponential form for this purpose, the Fisher-Rényi entropy product [17] and a new generalized LMC statistical complexity can be defined.

In this work, an information theoretical analysis of the same quantum system, the $H$-atom, is presented in terms of the Fisher-Rényi entropy product and the generalized LMC statistical measure. These $\alpha$-dependent magnitudes show a similar behavior to that found in the limit $\alpha \to 1$, that correspond to the already studied case of the Fisher-Shannon information and LMC complexity [7]. That is, the degeneration of the energy is also broken by these statistical magnitudes.

The paper is organized as follows. In section 2, the Fisher-Rényi entropy product is recalled and the generalized LMC complexity measure is introduced. Some of their properties are also presented. The calculation of these magnitudes in the $H$-atom is presented in section 3. Our conclusions are contained in the last section.
2. COMPLEXITY MEASURES

Consider a $D$-dimensional distribution function $f(r)$, with $f(r)$ nonnegative and $\int f(r) dr = 1$ and define Rényi entropy power of index $\alpha$ blue as in [17] by

$$N_f^{(\alpha)} = \frac{\eta_{\alpha}}{2\pi} \exp \left( \frac{2}{D} R_f^{(\alpha)} \right), \quad \text{with} \quad \alpha > \frac{1}{2},$$

being $\eta_{\alpha} = \left( \frac{\alpha}{2\alpha - 1} \right)^{2\alpha - 1}$ a decreasing function from 1 to 0 when $\alpha$ runs in $(0.5, \infty)$ and $\eta_{\alpha=1} = e^{-1}$, and the Rényi entropy of order $\alpha$ given by

$$R_f^{(\alpha)} = \frac{1}{1 - \alpha} \ln \int \left| f(r) \right|^\alpha dr,$$

where $r$ stands for $r_1, ..., r_D$.

Rényi entropy power is an extension of Shannon entropy power [18] and verifies that when $\alpha \to 1$ then $N_f^{(\alpha)} \to N_f = \frac{1}{2\pi e} e^{\frac{1}{2} S_f}$ with

$$S_f = -\int f(r) \ln f(r) dr.$$  \hspace{1cm} (3)

A scaling property is verified by Rényi entropy power [17], which transforms as

$$N_{|\Psi|^2}^{(\alpha)} = \lambda^{-2} N_{|\Psi|^2}^{(\alpha)},$$

under scaling of the function $\Psi_\lambda(r_1, ..., r_D) = \lambda^{D/2} \Psi(\lambda r_1, ..., \lambda r_D)$. Rényi entropy power also has the property [17]

$$N_f^{(\alpha)} > N_f^{(\alpha')}, \quad \text{for} \quad \alpha < \alpha'.$$  \hspace{1cm} (5)

Fisher information [19] of the probability density function $f$ is given by

$$I_f = \int \frac{|\nabla f(r)|^2}{f(r)} dr.$$  \hspace{1cm} (6)

### A. Fisher-Rényi Entropy Product $P_f^{(\alpha)}$

The Fisher-Rényi entropy product is defined by

$$P_f^{(\alpha)} = \frac{1}{D} N_f^{(\alpha)} I_f, \quad \text{with} \quad \alpha \in (1/2, 1].$$

It displays the following important properties [17]:

(i) $P_f^{(\alpha)}$ is invariant under scaling transformation $f_\lambda = \lambda^D f(\lambda r)$, i.e. $P_{f_\lambda}^{(\alpha)} = P_f^{(\alpha)}$,

(ii) it verifies the inequality $P_f^{(\alpha)} \geq 1$, and

(iii) $P_f^{(\alpha)}$ is a nonincreasing function of $\alpha$ for any probability density.
B. Generalized Complexity Measure \( C^{(\alpha)}_f \)

The measure of complexity \( C_f \) introduced in [11, 12], the so-called LMC complexity, is defined by

\[
C_f = H_f Q_f, \quad \text{with} \quad H_f = e^{S_f} \quad \text{and} \quad Q_f = e^{-R^{(2)}_f}.
\]

(8)

It can be generalized to the \( \alpha \)-dependent measure of complexity, \( C^{(\alpha)}_f \), which is defined by

\[
C^{(\alpha)}_f = H^{(\alpha)}_f Q_f, \quad \text{with} \quad H^{(\alpha)}_f = e^{R^{(\alpha)}_f},
\]

(9)

that tends to the measure of complexity \( C_f \) in the limit \( \alpha \to 1 \). It satisfies the next properties:

(i) \( C^{(\alpha=2)}_f = 1 \),

(ii) \( C^{(\alpha)}_f \) is invariant under scaling transformation, \( f_{\lambda} = \lambda^D f(\lambda r) \), i.e. \( C^{(\alpha)}_{f_{\lambda}} = C^{(\alpha)}_f \),

(iii) taking into account that Rényi entropy is a nonincreasing function of \( \alpha \) [18], it is straightforward to see that \( C^{(\alpha)}_f \geq 1 \) for \( \alpha < 2 \), \( C^{(\alpha)}_f \leq 1 \) for \( \alpha > 2 \), and \( C^{(\alpha)}_f \) is also a nonincreasing function of \( \alpha \).

Let us finally point out that when \( \alpha \) goes to 1, the lower bound (that takes the value 1) for the original LMC complexity is recovered [12].

3. CALCULATIONS ON THE HYDROGEN ATOM

The probability density, \( \rho(r) \), for a bound state, \( \Psi_{n\ell m}(r) \), with quantum numbers \((n, l, m)\) of the non-relativistic H-atom is given by \( \rho(r) = |\Psi_{n\ell m}(r)|^2 \) in position space \((r, \Omega)\) with \( r \) the radial distance and \( \Omega \) the solid angle), with

\[
\Psi_{n\ell m}(r) = R_{\ell m}(r)Y_{\ell m}(\Omega).
\]

(10)

The radial part, \( R_{\ell m}(r) \), is expressed as [20]

\[
R_{\ell m}(r) = \frac{2}{n^2} \left( \frac{(n - l - 1)!}{(n + l)!} \right)^{1/2} \left( \frac{2r}{n} \right)^l e^{-r/n} L^{2l+1}_{n-\ell-1} \left( \frac{2r}{n} \right),
\]

(11)

with \( L^n_\ell(r) \) the associated Laguerre polynomials, and \( Y_{\ell m}(\Omega) \) the spherical harmonic of the atomic state. Let us recall at this point the range of the quantum numbers: \( n \geq 1, 0 \leq l \leq n - 1 \), and \( -l \leq m \leq l \). Atomic units are used through the text.
Taking the density $\rho(r)$, we have calculated the Fisher-Rényi product $P^{(\alpha)}_\rho$ and the generalized complexity measure $C^{(\alpha)}_\rho$ for different $(n, l, m)$ wave functions of the $H$-atom.

In Figure 1, the entropy product $P^{(\alpha)}_\rho$ was computed numerically for $n = 15$ and $l = 5, 10, 14$ versus $|m|$ with $\alpha = 0.6$ (Fig. 1(a)) and $\alpha = 0.8$ (Fig. 1(b)). One can see that the minimum of this quantity is given when $l = n-1$. This behavior where the energy degeneracy is split by $P^{(\alpha)}_\rho$ is found for any energy level $n$, and also for any $\alpha$, with $0.5 < \alpha \leq 1$.

In Figure 2, the value of $C^{(\alpha)}_\rho$ is shown for $n = 15$ and $l = 5, 10, 14$ versus $|m|$ with $\alpha = 0.6$ (Fig. 2(a)), $\alpha = 1.5$ (Fig. 2(b)), and $\alpha = 2.5$ (Fig. 2(c)). As before, it can be seen that the minimum of $C^{(\alpha)}_\rho$ corresponds just to the highest $l$ when $0 < \alpha < 2$ (Figs. 2(a) and 2(b)), but for $\alpha > 2$ (Fig. 2(c)), we observe the opposite behavior, that is, the highest $l$ presents the maximum value of $C^{(\alpha)}_\rho$. So, a similar information is provided by both measures $C^{(\alpha)}_\rho$ when $0 < \alpha < 2$ and $P^{(\alpha)}_\rho$ when $0.5 < \alpha \leq 1$.

In Figure 3, the value of $C^{(\alpha)}_\rho$ is shown for $n = 15$ and $l = 5, 10, 14$ (and $0 \leq |m| \leq l$) versus $Q_\rho$ with $\alpha = 1.5$ (Fig. 3(a)) and $\alpha = 2.5$ (Fig. 3(b)). Let us observe in this figure the two possibilities of the property (iii) for the quantity $C^{(\alpha)}_\rho$. In Fig. 3(a), we have $\alpha = 1.5$, then $C^{(\alpha)} \geq 1$, and in Fig. 3(b), $\alpha = 2.5$, then $C^{(\alpha)} \leq 1$.

4. SUMMARY

When the Shannon information ingredient of the statistical complexity and the Fisher-Shannon entropy is substituted by the Rényi entropy of order $\alpha$, two $\alpha$-families of statistical measures are obtained. Some of their properties have been presented. Also, they have been calculated on the hydrogen atom taking advantage of the exact knowledge of its wave functions. We have put in evidence that, for a fixed level of energy $n$, these quantities, the generalized statistical complexity and Fisher-Rényi entropy product, take their minimum values for the highest allowed orbital angular momentum, $l = n − 1$. This behavior is displayed when $0 < \alpha < 2$ for the generalized statistical complexity, and when $0.5 < \alpha \leq 1$ for the Fisher-Rényi entropy product, just in the range where uncertainty relations have been shown for this indicator. When $\alpha > 2$, the opposite behavior is found for the generalized statistical complexity, i.e. the maximum of this quantity is taken on the highest angular momentum, and for the Fisher-Rényi entropy product, the last described behavior is lost when $\alpha > 1$. 

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We conclude by observing that the exchange of the Shannon information by the Rényi entropy of order $\alpha$ in the statistical complexity and Fisher-Shannon entropy still keeps the property of energy degeneracy breaking in the $H$-atom. Further work could be required in order to unveil if this feature is displayed in other quantum systems.
[1] S.R. Gadre, S.B. Sears, S.J. Chakravorty, and R.D. Bendale, Phys. Rev. A 32 (1985) 2602.
[2] K.Ch. Chatzisavvas, Ch.C. Moustakidis, and C.P. Panos, J. Chem. Phys. 123 (2005) 174111.
[3] R.J. Yáñez, W. van Assche, and J.S. Dehesa, Phys. Rev. A 50 (1994) 3065.
[4] M.W. Coffey, J. Phys. A: Math. Gen. 36 (2003) 7441.
[5] E. Romera, P. Sánchez-Moreno, and J.S. Dehesa, Chem. Phys. Lett. 414 (2005) 468.
[6] J. B. Szabo, K. D. Sen, and A. Nagy, Phys. Lett. A 372 (2008) 2428.
[7] J. Sañudo and R. López-Ruiz, Phys. Lett. A 372 (2008) 5283.
[8] C. Vignat, J. F. Bercher, Phys. Lett. A 312 (2003) 27.
[9] E. Romera and J. S. Dehesa, J. Chem. Phys. 120 (2004) 8906.
[10] J.C. Angulo, J. Antolín, and K.D. Sen, Phys. Lett. A 372 (2008) 670.
[11] R. López-Ruiz, H. L. Mancini, and X. Calbet, Phys. Lett. A 209 (1995) 321.
[12] R.G. Catalan, J. Garay, and R. López-Ruiz, Phys. Rev. E 66 (2002) 011102.
[13] C.E. Shannon, A mathematical theory of communication, Bell. Sys. Tech. J. 27 (1948) 379; ibid. (1948) 623.
[14] A. Rényi, Proceedings of the 4th Berkeley Symposium on Mathematical Statistics and Probability, Volume 1: Contributions to the Theory of Statistics (1961) 547.
[15] C. Tsallis, J. Stat. Phys. 52, (1988) 479.
[16] M.T. Martin, A. Plastino and O.A. Rosso, Physica A 369 (2006) 439.
[17] E. Romera and Á. Nagy, Phys. Lett. A 372 (2008) 6823.
[18] A. Dembo, T.M. Cover, and J.A. Thomas, IEEE Trans. Inf. Theor. 37 (1991) 1501.
[19] R.A. Fisher, Proc. Cambridge Phil. Soc. 22 (1925) 700.
[20] A. Galindo and P. Pascual, Quantum Mechanics I, Springer, Berlin, 1991.
FIG. 1: Fisher-Rényi entropy product in position space, $P_{\rho}^{(\alpha)}$ vs. $|m|$ for different $l$ values when $n = 15$ in the hydrogen atom. (a) $\alpha = 0.6$ and (b) $\alpha = 0.8$. All values are in atomic units.
FIG. 2: Generalized statistical complexity in position space, $C_{p}^{(\alpha)}$ vs. $|m|$ for different $l$ values when $n = 15$ in the hydrogen atom. (a) $\alpha = 0.6$, (b) $\alpha = 1.5$, and $\alpha = 2.5$. All values are in atomic units.
FIG. 3: Generalized statistical complexity in position space, $C^{(\alpha)}_\rho$ vs. $Q_\rho$ for different $l$ values when $n = 15$ and $0 \leq |m| \leq l$ in the hydrogen atom. (a) $\alpha = 1.5$ and (b) $\alpha = 2.5$. The dashed lines represent the lower bound (= 1) and the upper bound (= 1) for the $C^{(\alpha)}_\rho$, in the cases $0 < \alpha < 2$ and $\alpha > 2$, respectively. All values are in atomic units.