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Review

Cramér–Rao, Fisher–Shannon and LMC–Rényi Complexity-like Measures of Multidimensional Hydrogenic Systems with Application to Rydberg States

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Abstract: Statistical measures of complexity hold significant potential for applications in D-dimensional finite fermion systems, spanning from the quantification of the internal disorder of atoms and molecules to the information–theoretical analysis of chemical reactions. This potential will be shown in hydrogenic systems by means of the monotone complexity measures of Cramér–Rao, Fisher–Shannon and LMC(Lopez-Ruiz, Mancini, Calbet)–Rényi types. These quantities are shown to be analytically determined from first principles, i.e., explicitly in terms of the space dimensionality D, the nuclear charge and the hyperquantum numbers, which characterize the system' states. Then, they are applied to several relevant classes of particular states with emphasis on the quasi-spherical and the highly excited Rydberg states, obtaining compact and physically transparent expressions. This is possible because of the use of powerful techniques of approximation theory and orthogonal polynomials, asymptotics and generalized hypergeometric functions.

Keywords: multidimensional hydrogenic systems; Cramér–Rao complexity-like measures; Fisher–Shannon complexity-like measures; LMC–Rényi complexity-like measures; highly excited Rydberg states

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1. Introduction

The physical and chemical properties of atomic and molecular systems can be described, according to the density–functional theory, by means of integral functionals of the electron probability density $\rho(\mathbf{r})$ (see e.g., [1,2]). These functionals, which quantify the multifaceted electronic complexity of these systems, are obtained from the entropy-like and complexity-like (Cramér–Rao, Fisher–Shannon, LMC–Rényi) measures of the systems: the basic variables of the classical and quantum information and complexity theory [3,4]. The entropic measures of a multidimensional quantum system (Fisher, Shannon, Rényi) quantify, like the familiar variance, a single facet of $\rho(\mathbf{r})$; however, opposite to the variance, they do not depend on any particular point of the density's domain such that they are much more appropriate quantities for the uncertainty type.

The complexity-like measures estimate the combined balance of two or more facets of the density. Guided by the theory of quantum entanglement [5] and the recent developments of quantum coherence [6], we will here consider the most relevant monotone complexity-like measures [7] of a finite D-dimensional quantum system so that each simultaneously quantifies two facets of its internal disorder as described by the electron density $\rho(\mathbf{r})$, namely, the Cramér–Rao complexity [8], the Fisher–Shannon complexity [9–12] and the LMC–Rényi complexity [13–17]; see also some modifications of them [14–16,18–25].

In this work, we review and determine these complexity-like measures for the general quantum states of the D-dimensional hydrogenic system in terms of the state's hyperquantum numbers, the nuclear charge and the space dimensionality; each measure allows us to estimate jointly two different facets of the electronic complexity [26–30]. Then, we apply them to several relevant classes of particular states with emphasis on the quasi-spherical and highly excited Rydberg states. This hydrogenic system plays a fundamental role in the multidimensional quantum physics since encompasses a great deal of the standard three-dimensional hydrogenic atoms (see, for example, [31]) and non-standard low- and high-dimensional objects of great relevance in condensed matter, quantum cosmology and quantum computation, such as quantum wells, wires and dots, semiconductor excitons, qubits, Rydberg atoms, exotic atoms, and antimatter atoms, . . . (see, for example, [32–38]).

The Cramér–Rao complexity $C_{CR}[\rho]$ measures the gradient content of the electron density jointly with its concentration around the centroid. The Fisher–Shannon complexity $C_{FS}[\rho]$ quantifies the concentration of electron density around its maxima together with its total spreading all over the system's volume. The (biparametric) LMC–Rényi complexity $\overline{C}_{\alpha,\beta}[\rho]$ takes into account two different aspects of the electronic spreading of the system, which depend on the specific values of its two parameters. The particular case ($\alpha \to 1$, $\beta = 2$) corresponds to the plain LMC (López-Ruiz–Mancini–Calvet) complexity measure [15,39,40] $C_{1,2}[\rho]$ which quantifies the density's non-uniformity (or departure from equiprobability) jointly with its total extent over the density domain. These complexity-like measures were recently applied to numerous phenomena in atomic and molecular physics [24,28,29,41–50] and chemical reactions [51–53], and its analytical determination is shown to require powerful algebraic techniques [54–59] and asymptotical methods [60–64] of approximation theory and orthogonal polynomials.

The structure of the paper is the following. In Section 2, we fix the notation used and briefly define and discuss the monotonic complexity-like measures of a general multidimensional density considered in this work. In Section 3, we show and analyze the probability density of the multidimensional hydrogenic system in light of the complexity-like measures previously mentioned. In Sections 4–6, we describe the main results on the Crámer–Rao, Fisher–Shannon and LMC–Rényi complexity measures of the multidimensional hydrogenic systems, respectively, and we apply them to various specific states of quasi-spherical and highly excited Rydberg states. Finally, some concluding remarks are given.

2. Complexity-like Measures of a Multidimensional Density

In this section, we show the complexity-like measures of a D-dimensional quantum density $\rho(\mathbf{r})$ in position space which fulfills the monotonicity property [7]. They are the Cramér–Rao complexity measure [8,14,65] defined by

$$C_{CR}[\rho] := F[\rho] \times V[\rho] = F[\rho] \times \left\langle r^2 \right\rangle, \tag{1}$$

(the second equality holds for quantum systems subject to a central potential, because then the variance $V[\rho] = \langle r^2 \rangle$ as shown later on), the Fisher–Shannon complexity [9–12] given by

$$C_{FS}[\rho] := F[\rho] \times \frac{1}{2\pi e} e^{\frac{2}{D} S[\rho]}. \tag{2}$$

and their generalization, the LMC–Rényi complexity [13–16,19], defined as

$$\overline{C}_{\alpha,\beta}[\rho] := e^{\frac{1}{D}(R_\alpha[\rho] - R_\beta[\rho])}, \quad 0 < \alpha < \beta < \infty, \quad \alpha, \beta \neq 1, \tag{3}$$

where $F[\rho]$, $S[\rho]$ and $R_q[\rho]$ denote the Fisher information [66–68], the Shannon entropy [69,70] and Rényi entropy of order q [71,72], respectively. They are expressed as

$$F[\rho] := \int_{\mathbb{R}_D} \frac{|\nabla_D \rho(\mathbf{r})|^2}{\rho(\mathbf{r})} d\mathbf{r}, \tag{4}$$

$$S[\rho] := -\int_{\mathbb{R}_D} \rho(\mathbf{r}) \log \rho(\mathbf{r})\, d\mathbf{r}; \quad R_q[\rho] = \frac{1}{1-q} \log \int_{\mathbb{R}_D} [\rho(\mathbf{r})]^q\, d\mathbf{r}, \quad 0 < q < \infty,\, q \neq 1, \tag{5}$$

respectively, being $r \equiv |\mathbf{r}|$, $\mathbf{r} = (r, \theta_1, \theta_2, \ldots, \theta_{D-1}) \equiv (r, \Omega_{D-1})$, $d\mathbf{r} = r^{D-1} dr\, d\Omega_{D-1}$, with $d\Omega_{D-1} = \left(\prod_{j=1}^{D-2} \sin^{2\alpha_j} \theta_j\right) d\varphi$ and $2\alpha_j = D - j - 1$, and ∇_D the D-dimensional gradient operator given by

$$\nabla_D = \frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\sum_{i=1}^{D-2} \frac{\partial}{\partial \theta_i}\hat{\theta}_i + \frac{1}{r\prod_{i=1}^{D-2} \sin\theta_i}\frac{\partial}{\partial \varphi}\hat{\varphi}. \tag{6}$$

Symbol $\langle r^a \rangle = \int_{\mathbb{R}_D} r^a \rho(\mathbf{r}) d\mathbf{r}, a = 1, 2$ and the variance of the density is defined as the sum of variances of the components of $\mathbf{r}$ so that $V[\rho] = \int |\mathbf{r} - \langle \mathbf{r} \rangle|^2 \rho(\mathbf{r})\, d\mathbf{r} = \langle |\mathbf{r}|^2 \rangle - |\langle \mathbf{r} \rangle|^2 = \langle r^2 \rangle$, since $|\langle \mathbf{r} \rangle|^2 = 0$ for any quantum state of a central potential. Then the variance quantifies the concentration of the density around the origin. There is a certain controversy about the notion of variance [41,73–76]. For general quantum systems, it is often defined as $\langle r^2 \rangle - \langle r \rangle^2$; however, it corresponds to the one-dimensional radial density but not to the total multidimensional density. The Rényi entropies, which have very relevant properties [26,77–81], estimate numerous spreading-like facets of the quantum probability density, allowing for a quantitative discussion of the intrinsic randomness (quantum uncertainty) and the geometrical profile of the quantum system; so, further beyond the Heisenberg-like uncertainty [82,83] which is based on the variance of the density and their generalizations, the radial expectation values [84].

In addition, the limit $q \to 1$ allows to recover the Shannon entropy from the Rényi entropy, i.e., $\lim_{q\to 1} R_q[\rho] = S[\rho]$. Moreover, the case ($\alpha \to 1$, $\beta = 2$) of the LMC–Rényi complexity (3) describes the plain LMC (López-Ruiz–Mancini–Calvet) complexity measure [15,39,40] $C_{1,2}[\rho] = \mathcal{D}[\rho] \times e^{S[\rho]}$, which measures the combined balance of the density's departure from equiprobability (or disequilibrium $\mathcal{D}[\rho] = e^{-R_2[\rho]}$) and its total extent (as given by the power Shannon quantity $e^{S[\rho]}$). Moreover, the Fisher information is a local uncertainty measure [85] because it depends on the density's gradient operator so that it increases with the concentration of the density among its nodes; the Shannon and Rényi entropies are uncertainty measures of global character because they are logarithmic and power integral functionals of $\rho(\mathbf{r})$, which estimate different macroscopic aspects of the density all over its dimensional support according to the parameter q.

Consequently, the Cramér–Rao quantity is a complexity measure of local–global character which depends on a specific point of the systems (the origin); and the Fisher–Shannon and LMC–Rényi quantities are complexity measures of local–global and global–global character, respectively, which do not depend on any specific point.

These three complexity measures are known to be dimensionless, invariant under translation and scaling transformation [86,87], and universally bounded from below [27,28,88,89] as

$$C_{CR}[\rho] \geq D^2, \quad C_{FS}[\rho] \geq D, \quad and \quad \overline{C}_{\alpha,\beta}[\rho] \geq 1 \quad if \quad \alpha < \beta \tag{7}$$

for D-dimensional probability densities. The universal minimum bound D^2 for the Cramér–Rao complexity is reached by the (Gaussian) density associated with the ground state of the D-dimensional harmonic oscillator [26,76]. Moreover, the LMC–Rényi complexities [13] give their minimum value when applied to the uniform distribution (maximum disorder) with a bounded support. However, these complexity measures are not well defined when applied to the Dirac-delta distribution (maximum order), although this is something which can be easily cured [20]. Other extensions/modifications of these statistical complexities have been proposed, such as the Fisher–Rényi complexities [18,19,21–23] and the biparametric Cramér–Rao and Heisenberg–Rényi complexities [24], although they will be discussed separately elsewhere together with some atomic and cosmological applications. Finally, the corresponding complexity measures for the probability density $\gamma(\mathbf{p})$ in momentum space [17] will be denoted by $C_{CR}[\gamma]$, $C_{FS}[\gamma]$ and $\overline{C}_{\alpha,\beta}[\gamma]$, respectively.

3. The Multidimensional Hydrogenic System: The Probability Density

In this section, we fix the notation and describe the wavefunctions and the associated probability densities for the stationary states of the D-dimensional hydrogenic system in both position and momentum spaces. This system is a negatively charged particle moving around a positively charged core which electromagnetically binds it in its orbit. Atomic units (i.e., $\hbar = m_e = e = 1$) are used throughout the paper.

The Schrödinger equation of the D-dimensional hydrogenic system has the form

$$\left(-\frac{1}{2}\nabla_D^2 + \mathcal{V}(r)\right)\Psi(\mathbf{r}) = E\Psi(\mathbf{r}), \tag{8}$$

where $\mathbf{r} = (r, \theta_1, \theta_2, \ldots, \theta_{D-1})$ in hyperspherical units and $r \equiv |\mathbf{r}| \in [0, +\infty)$. The symbols ∇_D and $\mathcal{V}(r)$ denote the D-dimensional gradient operator and the Coulomb potential $\mathcal{V}(\mathbf{r}) = -\frac{Z}{r}$, respectively. It has been shown [4,90] that the wavefunctions of this system are characterized by the energies

$$E = -\frac{Z^2}{2\eta^2}, \qquad \eta = n + \frac{D-3}{2}; \qquad n = 1, 2, 3, \ldots, \tag{9}$$

and the associated eigenfunctions

$$\Psi_{n,l,\{\mu\}}(\mathbf{r}) = \mathcal{R}_{n,l}(r) \times \mathcal{Y}_{l,\{\mu\}}(\Omega_{d-1}), \tag{10}$$

where $(l, \{\mu\}) \equiv (l \equiv \mu_1, \mu_2, \ldots, \mu_{D-1})$ denote the hyperquantum numbers associated to the angular variables $\Omega_{d-1} \equiv (\theta_1, \theta_2, \ldots, \theta_{D-1})$, which may take all values consistent with the inequalities $l \equiv \mu_1 \geq \mu_2 \geq \cdots \geq |\mu_{D-1}| \equiv |m| \geq 0$. The radial part of the eigenfunction is given by

$$\mathcal{R}_{n,l}(r) = \left(\frac{2Z}{\eta}\right)^{\frac{D}{2}} \left(\frac{1}{2\eta}\right)^{1/2} \left[\frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}}\right]^{1/2} \tilde{\mathcal{L}}_{\eta-L-1}^{(2L+1)}(\tilde{r}) \tag{11}$$

where $\tilde{r} = \frac{2Z}{\eta} r$, L is

$$L = l + \frac{D-3}{2}, \qquad l = 0, 1, 2, \ldots \tag{12}$$

and the symbol $\tilde{\mathcal{L}}_k^{(\alpha)}(x)$ denotes the orthonormal Laguerre polynomial of degree k with respect to the weight $\omega_\alpha(x) = x^\alpha e^{-x}$ on the interval $[0, \infty)$ [91]. The angular part of the eigenfunction is given by the known hyperspherical harmonics $\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})$ [90,92,93], defined as

$$\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) \quad = \quad \mathcal{N}_{l,\{\mu\}} e^{im\phi} \times \prod_{j=1}^{D-2} \mathcal{C}_{\mu_j-\mu_{j+1}}^{(\alpha_j+\mu_{j+1})}(\cos\theta_j)(\sin\theta_j)^{\mu_{j+1}} \tag{13}$$

with $\alpha_j = (D - j - 1)/2$ and the normalization constant

$$\mathcal{N}_{l,\{\mu\}}^2 = \frac{1}{2\pi} \times \prod_{j=1}^{D-2} \frac{(\alpha_j + \mu_j)(\mu_j - \mu_{j+1})![\Gamma(\alpha_j + \mu_{j+1})]^2}{\pi\, 2^{1-2\alpha_j-2\mu_{j+1}}\Gamma(2\alpha_j + \mu_j + \mu_{j+1})}, \tag{14}$$

where the symbol $\mathcal{C}_n^{(\lambda)}(t)$ denotes the Gegenbauer polynomial of degree n and parameter λ. These hyperfunctions satisfy the orthonomalization condition satisfy the orthonomalization condition

$$\int_{\mathcal{S}_{D-1}} \mathcal{Y}_{l',\{\mu'\}}^*(\Omega_{D-1})\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})d\Omega_{D-1} = \delta_{l,l'}\delta_{\{\mu\},\{\mu'\}} \tag{15}$$

Then, the position probability density for a generic $(n, l, \{\mu\}) \equiv (n, l, \mu_2, \ldots, \mu_{D-1})$ state of the D-dimensional hydrogenic systems is

$$\rho_{n,l,\{\mu\}}(\mathbf{r}) = \left|\Psi_{n,l,\{\mu\}}(\mathbf{r})\right|^2 = \mathcal{R}^2_{n,l}(r) \times \left|\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})\right|^2. \tag{16}$$

which is normalized so that $\int \rho_{n,l,\{\mu\}}(\mathbf{r})\, d\mathbf{r} = 1$.

The probability density in momentum spaces $\gamma(\mathbf{p})$ is obtained by squaring the d-dimensional Fourier transform of the configuration eigenfunction, i.e., the momentum eigenfunction [4]:

$$\tilde{\Psi}_{n,l,\{\mu\}}(\mathbf{p}) = \mathcal{M}_{n,l}(p) \times \mathcal{Y}_{l\{\mu\}}(\Omega_{D-1}), \tag{17}$$

whose radial part is

$$\mathcal{M}_{n,l}(p) = \left(\frac{\eta}{Z}\right)^{d/2} (1+y)^{3/2} \left(\frac{1+y}{1-y}\right)^{\frac{d-2}{4}} \sqrt{\omega^*_{L+1}(y)}\, \tilde{\mathcal{C}}^{L+1}_{\eta-L-1}(y) \tag{18}$$

$$= \left(\frac{\eta}{Z}\right)^{\frac{D}{2}} K_{n,l} \frac{(\eta\tilde{p})^l}{(1+\eta^2\tilde{p}^2)^{L+2}} \mathcal{C}^{(L+1)}_{\eta-L-1}\left(\frac{1-\eta^2\tilde{p}^2}{1+\eta^2\tilde{p}^2}\right), \tag{19}$$

with $y = \frac{1-\eta^2\tilde{p}^2}{1-\eta^2\tilde{p}^2}$, $\tilde{p} = \frac{p}{Z}$ and the constant

$$K_{n,l} = 2^{2L+3}\left[\frac{(\eta - L - 1)!}{2\pi(\eta + L)!}\right]^{\frac{1}{2}} \Gamma(L+1)\eta^{\frac{1}{2}}. \tag{20}$$

Symbols $\mathcal{C}^{(\alpha)}_k(y)$ and $\tilde{\mathcal{C}}^{(\alpha)}_k(x)$ denote the orthogonal and orthonormal Gegenbauer polynomials with respect to the weight function $\omega^*_\alpha(x) = (1-x^2)^{\alpha-\frac{1}{2}}$ on the interval $[-1, +1]$ [91], respectively, so that and the symbol $\mathcal{C}^{(\alpha)}_k(y)$ denote the orthogonal Gegenbauer polynomial, related to the orthonormal one as [91]

$$\tilde{\mathcal{C}}^{(\alpha)}_k(y) = \left(\frac{k!(k+\alpha)\Gamma^2(\alpha)}{\pi 2^{1-2\alpha}\Gamma(2\alpha+k)}\right)^{1/2} \mathcal{C}^{(\alpha)}_k(y). \tag{21}$$

The momentum probability density for a generic $(n, l, \{\mu\}) \equiv (n, l \equiv \mu_1, \mu_2, \ldots, \mu_{D-1})$ state of the D-dimensional hydrogenic systems is

$$\gamma_{n,l,\{\mu\}}(\mathbf{p}) = \left|\tilde{\Psi}_{n,l,\{\mu\}}(\mathbf{p})\right|^2 = \mathcal{M}^2_{n,l}(p) \times \left[\mathcal{Y}_{l\{\mu\}}(\Omega_{D-1})\right]^2, \tag{22}$$

which is normalized so that $\int \gamma_{n,l,\{\mu\}}(\mathbf{p})\, d\mathbf{p} = 1$.

Now, we will show the analytical determinarion of the complexity measures which quantify the different facets of the electron complexity of the D-dimensional hydrogenic system in both position and momentum spaces.

4. Hydrogenic Cramér–Rao Complexity

In this section, we first calculate the Cramér–Rao complexity (1) for a generic stationary state $(n, l, \{\mu\}) \equiv (n, l, \mu_2, \ldots, \mu_{d-1})$ of the D-dimensional hydrogenic system in both position and momentum spaces; then, we apply it to the three-dimensional hydrogenic atom. We have to determine the variance and the Fisher information. In position space, we obtain the values

$$
\begin{aligned}
V[\rho_{n,l,\{\mu\}}] = \left\langle r^2 \right\rangle &\equiv \int_{\mathbb{R}_D} r^2 \rho_{n,l,\{\mu\}}(\mathbf{r}) d\mathbf{r} = \int_0^\infty r^{d+1} \mathcal{R}_{nl}^2(r) dr \\
&= \frac{1}{2\eta}\left(\frac{\eta}{2}\right)^2 \int_0^\infty \omega_{2L+1}(\tilde{r}) \left[\tilde{\mathcal{L}}_{n_r}^{(2L+1)}(\tilde{r})\right]^2 \tilde{r}^3 d\tilde{r} \\
&= \frac{\eta^2}{2Z^2}\left[5\eta^2 - 3L(L+1) + 1\right], \qquad (23)
\end{aligned}
$$

and

$$
\begin{aligned}
F\left[\rho_{n,l,\{\mu\}}\right] &= \int_{\mathbb{R}_D} \frac{\left|\nabla_D \, \rho_{n,l,\{\mu\}}(\mathbf{r})\right|^2}{\rho_{n,l,\{\mu\}}(\mathbf{r})} d\mathbf{r} \\
&= 4\left\langle p^2 \right\rangle - 2|m|(2l + D - 2)\left\langle r^{-2} \right\rangle \\
&= \frac{4Z^2}{\eta^3}[\eta - |m|], \qquad D \geq 2. \qquad (24)
\end{aligned}
$$

for the variance [4,94,95] and the Fisher information [68,96,97] of the D-dimensional hydrogenic system, respectively. Here, we have also used that $\langle r^{-2} \rangle = \frac{2Z^2}{\eta^3}\frac{1}{2L+1}$. Then, the position Cramér–Rao complexity (1) for a generic D-dimensional hydrogenic state $(n, l, \mu_2, \ldots, \mu_{d-1})$ has the value

$$
C_{CR}[\rho_{n,l,\{\mu\}}] := F[\rho_{n,l,\{\mu\}}] \times V[\rho_{n,l,\{\mu\}}] = \frac{2}{\eta}(\eta - |m|)\,[5\eta^2 - 3L(L+1) + 1], \qquad (25)
$$

where η and L are given by Equations (9) and (12), respectively.

In momentum space, we can work in a similar manner. Then, we obtain the values

$$
V[\gamma_{n,l,\{\mu\}}] \quad = \langle p^2 \rangle = \int p^2 \gamma(\mathbf{p})\, d\mathbf{p} = \int_0^\infty p^{D+1} \mathcal{M}_{n,l}^2(p)\, dp \quad = \frac{Z^2}{\eta^2} \qquad (26)
$$

and

$$
\begin{aligned}
F\left[\gamma_{n,l,\{\mu\}}\right] &= 4\left\langle r^2 \right\rangle - 2|m|(2l + D - 2)\left\langle p^{-2} \right\rangle \\
&= \frac{2\eta^2}{Z^2}\left[5\eta^2 - 3L(L+1) - |m|(8\eta - 6L - 3) + 1\right]; \qquad D \geq 2. \qquad (27)
\end{aligned}
$$

for the variance [4,95,98–100] and Fisher information [68,96,97], where we have also used that $\langle p^{-2} \rangle = \frac{\eta^2}{Z^2}\frac{8\eta - 3(2L+1)}{2L+1}$. Then, the momentum Cramér–Rao complexity (1) has the value

$$
\begin{aligned}
C_{CR}[\gamma_{n,l,\{\mu\}}] &= F[\gamma_{n,l,\{\mu\}}] \times V[\gamma_{n,l,\{\mu\}}] \\
&= 2\left[5\eta^2 - 3L(L+1) - |m|(8\eta - 6L - 3) + 1\right] \qquad (28)
\end{aligned}
$$

for a generic D-dimensional hydrogenic state $(n, l, \mu_2, \ldots, \mu_{D-1})$. Note that the position and momentum Cramér–Rao complexity measures given by Equations (25) and (28) do not depend on the nuclear charge Z [101]; moreover, they are bigger than the universal minimum values D^2 (see Equation (7)) and $4\left[1 - \frac{2|m|}{2L+1}\right]\left(L + \frac{3}{2}\right)^2$ (see [102]) for the corresponding measures of general systems and systems with central potentials, respectively, as they should be.

The application of the previous general results (25) and (28) to quasi-spherical states (i.e., states with hyperangular momentum quantum numbers $\mu_1 = \mu_2 = \cdots = \mu_{d-1} = n-1$) gives rise to the following values:

$$C_{CR}[\rho_{n,n-1,\{n-1\}}] = \frac{(D-1)(2n+D-1)(2n+D-2)}{(2n+D-3)}, \tag{29}$$

$$C_{CR}[\gamma_{n,n-1,\{n-1\}}] = (2n+D)(D-1)+2, \tag{30}$$

for the Cramér–Rao complexity measures in position and momentum spaces, respectively.

In addition, for $D = 3$ we have from the general expressions (25) and (28) that the Cramér–Rao complexity for the stationary states (n,l,m) of the hydrogenic atom has the values [41,46]

$$C_{CR}[\rho_{n,l,m}] = \frac{2}{n}(5n^2 - 3l(l+1)+1)(n-|m|) \tag{31}$$

and

$$C_{CR}[\gamma_{n,l,m}] = 2(5n^2 - 3l(l+1) - |m|(8n-6l-3)+1), \tag{32}$$

in the position and momentum spaces, respectively. These expressions show that the Cramér–Rao complexity behaves as $10n^2$ for the highly excited Rydberg states (i.e., states with large n) of the hydrogenic atom with l fixed in both reciprocal spaces. See [89] for a numerical study of this complexity measure in some states of the three-dimensional hydrogen atom.

5. Hydrogenic Fisher-Shannon Complexity

In this section, we consider the Fisher–Shannon complexity (2) for a generic stationary state $(n,l,\{\mu\}) \equiv (n,l,\mu_2,\ldots,\mu_{d-1})$ of the D-dimensional hydrogenic system in both position and momentum spaces; then, we apply it to the three-dimensional hydrogenic atom. Emphasis is placed on the quasi-spherical and highly excited Rydberg hydrogenic states. According to (2), the position and momentum Fisher–Shannon complexity measures of general states $(n,l,\{\mu\})$ are given by

$$\begin{aligned} C_{FS}[\rho_{n,l,\{\mu\}}] &= F[\rho_{n,l,\{\mu\}}] \times \tfrac{1}{2\pi e} e^{\frac{2}{D}S[\rho_{n,l,\{\mu\}}]} \\ &= \tfrac{2}{\pi e \eta^3}[\eta - |m|] \times e^{\frac{2}{D}S[\rho_{n,l,\{\mu\}}]} \end{aligned} \tag{33}$$

and

$$\begin{aligned} C_{FS}[\gamma_{n,l,\{\mu\}}] &= F[\gamma_{n,l,\{\mu\}}] \times \frac{1}{2\pi e} e^{\frac{2}{D}S[\gamma_{n,l,\{\mu\}}]} \\ &= \frac{\eta^2}{\pi e}\Big[5\eta^2 - 3L(L+1) - |m|(8\eta - 6L - 3) + 1\Big] \times e^{\frac{2}{D}S[\gamma_{n,l,\{\mu\}}]}, \end{aligned} \tag{34}$$

respectively, where we have taken into account the values (24) and (27) for the position and momentum Fisher information. So, we need to calculate only the Shannon entropy for any hydrogenic state $(n,l,\{\mu\})$ in the two reciprocal spaces. In position space, the Shannon entropy [103] is

$$\begin{aligned} S[\rho_{n,l,\{\mu\}}] &= -\int_{\mathbb{R}_D} \rho_{n,l,\{\mu\}}(\mathbf{r}) \log \rho_{n,l,\{\mu\}}(\mathbf{r})\, d\mathbf{r} \\ &= S[\mathcal{R}_{n,l}, D] + S[\mathcal{Y}_{l,\{\mu\}}, D], \end{aligned} \tag{35}$$

where the radial and angular components, according to Equation (16), are given by

$$S[\mathcal{R}_{n,l}, D] = -\int_0^\infty r^{D-1}\mathcal{R}_{nl}^2(r)\, \log\left(\mathcal{R}_{nl}^2(r)\right) dr \tag{36}$$

and

$$S[\mathcal{Y}_{l,\{\mu\}}, D] = -\int_{\mathcal{S}_{D-1}} |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2 \log |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2 \, d\Omega_{D-1} \tag{37}$$

respectively. The entropy-like integral of the hyperspherical harmonics $S[\mathcal{Y}_{l,\{\mu\}}, D]$ is under control since it can be numerically evaluated by the efficient Buyarov et al.'s algorithm [104] and analytically calculated not only in some specific cases (see [105]) but also for arbitrary states as explained later on. Similarly, the momentum Shannon entropy is given by

$$\begin{aligned} S[\gamma_{n,l,\{\mu\}}] &= -\int_{\mathbb{R}_D} \gamma_{n,l,\{\mu\}}(\mathbf{p}) \log \gamma_{n,l,\{\mu\}}(\mathbf{p}) \, d\mathbf{p} \\ &= S[\mathcal{M}_{n,l}, D] + S[\mathcal{Y}_{l,\{\mu\}}, D], \end{aligned} \tag{38}$$

where the radial component, according to Equation (22), is given by

$$S[\mathcal{M}_{n,l}, D] = -\int_0^\infty p^{D-1} \mathcal{M}_{nl}^2(p) \, \log \left(\mathcal{M}_{nl}^2(p) \right) dp \tag{39}$$

Note that the two position and momentum radial Shannon components depend on the hyperquantum numbers $\{n, l \equiv \mu_1\}$ only, while the angular part does not depend on the principal hyperquantum number n, but only on the magnetic hyperquantum numbers $\{\mu_i, i = 1, \ldots, D-1\}$. Moreover, the radial and angular Shannon entropies can be determined [4] in terms of the entropy-like functionals of Laguerre and Gegenbauer polynomials, being that the expression

$$E_i[p_n] = -\int_0^\infty x^i \omega(x) p_n^2(x) \log p_n^2(x) dx, \quad i = 0, 1 \tag{40}$$

is the entropy-like functional of the polynomials $p_n(x)$ orthogonal with respect to the weight function $\omega(x)$. Indeed, according to Equations (11) and (36), we have that the radial position Shannon entropy is

$$S[\mathcal{R}_{n,l}, D] = A(n, l, D) + \frac{1}{2\eta} E_1\left[\tilde{\mathcal{L}}_{\eta-L-1}^{(2L+1)} \right] - D \log Z \tag{41}$$

with

$$A(n, l, D) = -2l \left[\frac{2\eta - 2L - 1}{2\eta} + \psi(\eta + L + 1) \right] + \frac{3\eta^2 - L(L+1)}{\eta} + -\log \left[\frac{2^{D-1}}{\eta^{D+1}} \right]. \tag{42}$$

And, according to Equations (18) and (39), the radial momentum Shannon entropy is

$$S[\mathcal{M}_{n,l}, D] = F(n, l, D) + E_0\left[\tilde{\mathcal{C}}_{\eta-L-1}^{(L+1)} \right] + D \log Z \tag{43}$$

where

$$\begin{aligned} F(n, l, D) = &-\log \frac{\eta^D}{2^{2L+4}} - (2L+4)[\psi(\eta + L + 1) - \psi(\eta)] \\ &+ \frac{L+2}{\eta} - (D+1)\left[1 - \frac{2\eta(2L+1)}{4\eta^2 - 1} \right], \end{aligned} \tag{44}$$

where $\psi(x)$ is the digamma or Psi function [91]. In addition, the angular component of the Shannon entropies (37) turns out to be [4,106]

$$S[\mathcal{Y}_{l,\{\mu\}}, D] = B(l, \{\mu\}, D) + \sum_{j=1}^{D-2} E_0\left[\tilde{\mathcal{C}}_{\mu_j - \mu_{j+1}}^{(\alpha_j + \mu_{j+1})} \right], \tag{45}$$

with the coefficient

$$B(l,\{\mu\},D) = \log(2\pi) - 2\sum_{j=1}^{D-2}\mu_{j+1}\Big[\psi(2\alpha_j+\mu_j+\mu_{j+1}) \\ -\psi(\alpha_j+\mu_j) - log\,2 - \frac{1}{2(\alpha_j+\mu_j)}\Big], \tag{46}$$

Following (33) and (34) and (41)–(45), the final expressions of position and momentum Fisher–Shannon complexity measures for any D-dimensional hydrogenic state $(n,l,\{\mu\}) \equiv (n,l,\mu_2,\ldots,\mu_{d-1})$ are given by Equations (33) and (34) with the following expressions for the position and momentum Shannon entropies:

$$S\Big[\rho_{n,l,\{\mu\}}\Big] = A(n,l,D) + B(l,\{\mu\},d) + \frac{1}{2\eta}E_1\Big[\tilde{\mathcal{L}}^{(2L+1)}_{\eta-L-1}\Big] + \sum_{j=1}^{D-2}E_0\Big[\tilde{\mathcal{C}}^{(\alpha_j+\mu_{j+1})}_{\mu_j-\mu_{j+1}}\Big] - D\log Z, \tag{47}$$

and

$$S\Big[\gamma_{n,l,\{\mu\}}\Big] = F(n,l,D) + B(l,\{\mu\},D) + E_0\Big[\tilde{\mathcal{C}}^{(L+1)}_{\eta-L-1}\Big] + \sum_{j=1}^{D-2}E_0\Big[\tilde{\mathcal{C}}^{(\alpha_j+\mu_{j+1})}_{\mu_j-\mu_{j+1}}\Big] + D\log Z, \tag{48}$$

respectively. Recently, these two entropy-like functionals of Laguerre and Gegenbauer polynomials were encountered by the use of some linearization techniques of orthonormal polynomials such that analytical compact expressions were found for the position and momentum Shannon entropies (and then for the corresponding Fisher–Shannon complexity measures) [107], which can be symbolically solved by general-purpose computer algebra systems, such as Maple and Mathematica and their variations [108,109].

5.1. Application to Quasi-Spherical and Ground States

The application of the previous result to the quasi-spherical states, $(n, n-1, \{n-1\}) = (n, \mu_1 = \mu_2 \ldots = \mu_{D-1} = n-1)$, of the D-dimensional hydrogenic system with nuclear charge Z allowed us to find [29] the following values:

$$S[\rho_{n,n-1,\{n-1\}}] = D\,\log\left(\frac{e\sqrt{\pi}\,\eta}{2}\right) + \log\left(\frac{2\,\Gamma(2\,\eta+1)}{(n)_{\frac{D}{2}-1}}\right) + (n-1)\,c_{D,n} - D\log Z, \tag{49}$$

for the position Shannon entropy, with $\eta = n + \frac{D-3}{2}$ and $c_{D,n} = \psi(\eta+\frac{1}{2}) - \psi(n) - 2\psi(2\eta+1)+2$. And for $n=1$ one has the value

$$S[\rho_{1,0,\{0\}}] = D\,\log\left(\frac{e\sqrt{\pi}}{4}\right) + \log\left(\frac{2\,(D-1)^D\,\Gamma(D)}{\Gamma\left(\frac{D}{2}\right)}\right) - D\log Z,$$

for the position Shannon entropy for the ground state $(n,l,\{\mu\}) = (1,0,\{0\})$ of the D-dimensional hydrogenic system with nuclear charge Z. Moreover, for three dimensional hydrogenic systems, we have the values

$$S[\rho_{n,n-1,n-1}, D=3] = \log\Big[\pi\Gamma(n)^2 n^4\Big] + 2n + \frac{1}{n} - (2n-2)\psi(n) - 3\log Z$$

$$S[\rho_{1,0,0}, D=3] = 3 + \log\pi - 3\log Z \tag{50}$$

for the position Shannon entropies of the quasi-circular states and the ground state, respectively. Then, for example, from (33) and (50), we have the value $C_{FS}[\rho_{1,0,0}, D=3] = \frac{2e}{\pi^{1/3}}$ for the Fisher–Shannon complexity of the three-dimensional hydrogenic atom.

Similarly, we can find [29] that the momentum Shannon entropy for the quasi-spherical states, $(n, n-1, \{n-1\}) = (n, \mu_1 = \mu_2 \ldots = \mu_{D-1} = n-1)$, of the D-dimensional hydrogenic system with nuclear charge Z is given by

$$S\left[\gamma_{n,n-1,\{n-1\}}\right] = A(n,D) + \log\left[\frac{2^{D+1}\pi^{\frac{D+1}{2}}\Gamma(n)}{(2n+D-3)^D\Gamma\left(n+\frac{D-1}{2}\right)}\right] + D\log Z, \quad (51)$$

where the constant

$$A(n,D) = \frac{2n+D-1}{2n+D-3} - \frac{D+1}{2n+D-2} - (n-1)\psi(n) - \left(\frac{D+1}{2}\right)\psi\left(n+\frac{D-2}{2}\right) + \left(n+\frac{D-1}{2}\right)\psi\left(n+\frac{D-3}{2}\right). \quad (52)$$

For the particular case $n=1$, one has the value

$$S\left[\gamma_{1,0,\{0\}}\right] = \log\frac{\pi^{\frac{D+1}{2}}}{(D-1)^D\Gamma\left(\frac{D+1}{2}\right)} + (D+1)\left[\psi(D+1) - \psi\left(\frac{D}{2}+1\right)\right] + D\log Z, \quad (53)$$

for the momentum Shannon entropy of the ground state.

Finally, the corresponding position and momentum Fisher–Shannon complexity measures for the quasi-spherical and ground states are given by Equations (33) and (34) together with the Shannon entropy values (51) and (53), respectively. A numerical study of these complexity measures is conducted in [41,110] for a few specific three-dimensional hydrogenic states.

5.2. Application to Highly Excited Rydberg States

The position and momentum Fisher–Shannon complexity measures for the highly excited Rydberg states (i.e., states $(n, l, \{\mu\})$ with $n \to \infty$) are given by Equations (33) and (34), respectively, together with the Shannon entropy values:

$$S^{(Ry)}\left[\rho_{n,l,\{\mu\}}\right] = 2D\log n + (2-D)\log 2 + \log\pi + D - 3 - D\log Z + S\left(\mathcal{Y}_{l,\{\mu\}}\right) + o(1) \quad (54)$$

in position space [4,111] (see also [41,112] for three-dimensional systems), and

$$S^{(Ry)}[\gamma_{n,l,\{\mu\}}] = -D\log n + D\log Z + 5\log 2 - D - 2 + \log\pi + S[\mathcal{Y}_{l,\{\mu\}}] + O(\frac{1}{n}) \quad (55)$$

in momentum space [113], which improves a previously known result [4,41]. The proof of these results requires the use of the strong (degree) asymptotics of the entropy-like functionals of the Laguerre and Gegenbauer orthogonal polynomials, which control the wavefunctions of the Rydberg states in both position and momentum spaces, in the spirit of Aptekarev et al. [60,61,114–117]. In particular, for the Rydberg (nS)-states, we have the following values:

$$S^{(Ry)}\left[\rho_{n,0,\{0\}}\right] = 2D\log n + (2-D)\log 2 + 2\log\pi + D - 3 + o(1), \quad (56)$$

for the position Shannon entropy [41], and

$$S^{(Ry)}[\gamma_{n,0,\{0\}}] = -D\log n + D\log Z + 6\log 2 - D - 2n + (\frac{D}{2}+1)\log\pi - \log\Gamma(\frac{D}{2}) + O(\frac{1}{n}) \quad (57)$$

for the momentum Shannon entropy [113], where we have used that the angular Shannon entropy $S[\mathcal{Y}_{0,\{0\}}] = \log 2 + \frac{D}{2}\log\pi - \log\Gamma(\frac{D}{2})$.

Finally, one has from (54) and (55) that the total Shannon-entropy uncertainty for the Rydberg D-dimensional hydrogenic state $(l, \{\mu\})$ is given by the sum

$$S^{(Ry)}\left[\rho_{n,l,\{\mu\}}\right] + S^{(Ry)}\left[\gamma_{n,l,\{\mu\}}\right] = D\log n + (7-D)\log 2 + 2\log \pi - 5 + 2\,S\left(\mathcal{Y}_{l,\{\mu\}}\right) + o(1). \quad (58)$$

So that the net sum of the position and momentum Shannon uncertainties follows a $D\log n$ law. In addition, it does not depend on the nuclear charge Z because of the homogeneity of the Coulomb potential [90,101]. Let us also highlight that this entropic uncertainty sum satisfies not only the universal entropic uncertainty relation [118], $S[\rho] + S[\gamma] \geq D(1+\log \pi)$, but also the more stringent entropic uncertainty sum [119]

$$S[\rho] + S[\gamma] \geq B_{l,\{\mu\}} \quad (59)$$

with

$$B_{l,\{\mu\}} = 2l + D + 2\log\left[\frac{\Gamma\left(l+\frac{D}{2}\right)}{2}\right] - (2l+D-1)\,\psi\left(l+\frac{D}{2}\right) + (D-1)\left(\psi\left(\frac{2l+D}{4}\right) + \log 2\right) + 2S(\mathcal{Y}_{l,\{\mu\}}) \quad (60)$$

valid for the spherically symmetric quantum states. Notice that this bound depends on the magnetic hyperquantum numbers $(l, \{\mu\})$ and the dimensionality D, but not on the principal (energetic) quantum number n because the analytical form of the central potential $V_D(r)$ was not specified.

Then, for example, the Fisher–Shannon complexity of the three-dimensional Rydberg states (n, l, m) with $n \to \infty$ and (l, m) fixed has the following value:

$$C^{(Ry)}_{FS}[\rho_{n,l,m}] = \left(\frac{2}{\pi}\right)^{\frac{1}{3}} e^{-1+\frac{2}{3}S(Y_{l,m})} n^2 + o(n^2), \quad (61)$$

according to (33), (54) and (55). The symbol $S(Y_{l,m})$ denotes the angular Shannon entropy, which is under control as already discussed. In particular, for states with $|m| = l$, one has

$$S(Y_{l,l}) = \log\left(\frac{2^{2l+1}\pi^{\frac{3}{2}} l!}{\Gamma(l+\frac{3}{2})}\right) - 2l\left[\psi(2l+1) - \psi\left(l+\frac{1}{2}\right) - \frac{1}{2l+1}\right], \quad (62)$$

and for $nS-$states (i.e., when $l = m = 0$), one has that $S(Y_{0,0}) = \log 4\pi$. In the case that l is not fixed, as it often happens, then the expression (61) varies because then the involved Laguerre polynomial is a varying polynomial and consequently, the position Shannon entropy is not (54) anymore but one has to take into account the values found by [120].

6. Hydrogenic LMC-Rényi Complexity

In this section, we consider the LMC–Rényi complexity (3) for a generic stationary state $(n, l, \{\mu\}) \equiv (n, l, \mu_2, \ldots, \mu_{d-1})$ of the D-dimensional hydrogenic system in both position and momentum spaces; then, we apply it to quasi-spherical and highly excited Rydberg hydrogenic states. According to (3), the LMC–Rényi complexity measures of the state $(n, l, \{\mu\})$ are given [13–17] by

$$\overline{C}_{\alpha,\beta}[\rho_{n,l,\{\mu\}}] := e^{\frac{1}{D}(R_\alpha[\rho_{n,l,\{\mu\}}] - R_\beta[\rho_{n,l,\{\mu\}}])}, \quad 0 < \alpha < \beta < \infty, \quad \alpha, \beta \neq 1, \quad (63)$$

and

$$\overline{C}_{\alpha,\beta}[\gamma_{n,l,\{\mu\}}] := e^{\frac{1}{D}(R_\alpha[\rho_{n,l,\{\mu\}}] - R_\beta[\gamma_{n,l,\{\mu\}}])}, \quad 0 < \alpha < \beta < \infty, \quad \alpha, \beta \neq 1, \quad (64)$$

in the position and momentum spaces, respectively. The symbols $R_q[\rho_{n,l,\{\mu\}}]$ and $R_q[\gamma_{n,l,\{\mu\}}]$ (with natural q other than unity) denote the position and momentum Rényi entropies (5) of the D-dimensional hydrogenic states $(n, l, \{\mu\})$ respectively, given (see [121]) by

$$R_q[\rho_{n,l,\{\mu\}}] = \frac{1}{1-q} \log \int_{\mathbb{R}_D} [\rho_{n,l,\{\mu\}}(\mathbf{r})]^q \, d\mathbf{r} \tag{65}$$

$$= R_q[\mathcal{R}_{n,l}, D] + R_q[\mathcal{Y}_{l,\{\mu\}}] \tag{66}$$

in position space and

$$R_q[\gamma_{n,l,\{\mu\}}] = \frac{1}{1-q} \log \int_{\mathbb{R}_D} [\gamma_{n,l,\{\mu\}}(\mathbf{p})]^q \, d\mathbf{p} \tag{67}$$

$$= R_q[\mathcal{M}_{n,l}, D] + R_q[\mathcal{Y}_{l,\{\mu\}}] \tag{68}$$

in momentum space. Here the symbols $R_q[\mathcal{R}_{n,l}, D]$ and $R_q[\mathcal{M}_{n,l}, D]$ denote the position and momentum radial Rényi entropies respectively, given by

$$R_q[\mathcal{R}_{n,l}, D] = \frac{1}{1-q} \ln \int_0^\infty [\mathcal{R}_{n,l}(r)]^{2q} r^{D-1} \, dr \tag{69}$$

$$= \frac{1}{1-q} \ln\left[\left(\frac{\eta}{2Z}\right)^{D(1-q)} \left(\frac{\Gamma(n-l)}{2\eta\Gamma(n+l+D-2)} \right)^q \right]$$

$$+ \frac{1}{1-q} \ln q^{-D-2lq} \int_0^\infty x^{2lq+D-1} e^{-x} \left[\mathcal{L}_{n-l-1}^{(2l+D-2)}\left(\frac{x}{q}\right) \right]^{2q} dx, \tag{70}$$

(where we took into account (11) in the second equality) and

$$R_q[\mathcal{M}_{n,l}, D] = \frac{1}{1-q} \ln \int_0^\infty [\mathcal{M}_{n,l}(p)]^{2q} p^{D-1} \, dp \tag{71}$$

$$= \frac{1}{1-q} \ln\left(\frac{Z^D}{\eta^D} \frac{K_{n,l}^{2q}}{2^{q(L+2)}} \right) + \frac{1}{1-q} \times$$

$$\ln \int_{-1}^{1} (1-y)^{lq+\frac{D}{2}-1} (1+y)^{D(q-\frac{1}{2})+q(l+1)-1} \left[\mathcal{C}_{n-l-1}^{(L+1)}(y) \right]^{2q} dy \tag{72}$$

where we took into account (19) in the second equality; the constant $K_{n,l}$ is given by (20).

The symbol $R_q[\mathcal{Y}_{l,\{\mu\}}]$ in Equations (66) and (68) denotes the angular Rényi entropy given by

$$R_q[\mathcal{Y}_{l,\{\mu\}}] := \frac{1}{1-q} \ln \Lambda_q[\mathcal{Y}_{l,\{\mu\}}] \tag{73}$$

with the integral functionals of the hyperspherical harmonics [122] defined as

$$\Lambda_q[\mathcal{Y}_{l,\{\mu\}}] = \int_{\mathcal{S}_{D-1}} |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^{2q} \, d\Omega_{D-1}$$

$$= 2\pi \mathcal{N}_{l,\{\mu\}}^{2q} \prod_{j=1}^{D-2} \int_0^\pi [\mathcal{C}_{\mu_j-\mu_{j+1}}^{(\alpha_j+\mu_{j+1})}(\cos\theta_j)]^{2q} (\sin\theta_j)^{2q\mu_{j+1}+2\alpha_j} \, d\theta_j, \tag{74}$$

where the constant $\mathcal{N}_{l,\{\mu\}}$ is given by (14). Note that the angular Rényi entropies $R_q[\mathcal{Y}_{l,\{\mu\}}]$ do not depend on the principal hyperquantum number n.

Then, from Equations (69)–(74), we observe that the determination of the position and momentum radial and angular Rényi entropies of the D-dimensional hydrogenic systems are expressed in terms of some integral functionals of $(2q)$-type powers of Laguerre and Gegenbauer polynomials. These functionals were determined by use of the recent linearization techniques of hypergeometric orthogonal polynomials (Laguerre, Jacobi, Gegenbauer) [54–56] (see also [57]) together with some multivariate hypergeometric functions of Lauricella and Srivastava–Karlson types [55,58] .

The application of these techniques to the Laguerre and Gegenbauer functionals of (70) and (74) together with Equation (66) has allowed us to find [56,121] the position Rényi entropies of the D-dimensional hydrogenic states $(n, l, \{\mu\})$ as

$$\begin{aligned} R_q[\rho_{n,l,\{\mu\}}] &= D \ln\left(\frac{\pi^{\frac{1}{2}}\eta}{2Z}\right) + \frac{q}{1-q}\ln\left(\frac{(\eta-L)_{2L+1}}{2\eta}\right) \\ &+ \frac{1}{1-q}\ln\left[\mathcal{F}_q(D,\eta,L)\,\mathcal{A}_q(D,L)\right] + \frac{1}{1-q}\ln\left[\frac{\Gamma(l+\frac{D}{2})^q}{\Gamma\left(ql+\frac{D}{2}\right)}\frac{\Gamma(qm+1)}{\Gamma(m+1)^q}\right] \\ &+ \frac{1}{1-q}\sum_{j=1}^{D-2}\ln\left[\mathcal{B}_q(D,\mu_j,\mu_{j+1})\;\mathcal{G}_q(D,\mu_j,\mu_{j+1})\right] + \ln 2, \end{aligned} \tag{75}$$

with $\mathcal{A}_q(D,L) \equiv \frac{\Gamma(D+2lq)}{q^{D+2lq}\Gamma(2L+2)^{2q}}$, and

$$\mathcal{F}_q(D,n,l) \equiv F_A^{(2q)}\left(\begin{array}{c} 2lq+D;\overbrace{-n+l+1,\ldots,-n+l+1}^{2q} \\ \underbrace{2l+D-1,\ldots,2l+D-1}_{2q} \end{array};\underbrace{\frac{1}{q},\ldots,\frac{1}{q}}_{2q}\right), \tag{76}$$

where the symbol $F_A^{(s)}(x_1,\ldots,x_r)$ denotes the Lauricella function of type A of s variables and $2s+1$ parameters defined [59] as

$$F_A^{(s)}\left(\begin{array}{c} a;b_1,\ldots,b_s \\ c_1,\ldots,c_s \end{array};x_1,\ldots,x_s\right) = \sum_{j_1,\ldots,j_s=0}^{\infty}\frac{(a)_{j_1+\ldots+j_s}(b_1)_{j_1}\cdots(b_s)_{j_s}}{(c_1)_{j_1}\cdots(c_s)_{j_s}}\frac{x_1^{j_1}\cdots x_s^{j_s}}{j_1!\cdots j_s!}. \tag{77}$$

Note that the function $\mathcal{F}_q(D,n,l)$ is a finite sum because of the properties of the involved Pochhammer symbols $(z)_k = \frac{\Gamma(z+k)}{\Gamma(z)}$ with negative integer arguments. Moreover, for $l = n-1$ the function $\mathcal{F}_q(D,n,l)$ in Equation (76) is equal to unity such that the third term on the right side vanishes.

The symbols $B_q(D,\mu_j,\mu_{j+1})$ and $G_q(D,\mu_j,\mu_{j+1})$ denote the values

$$\mathcal{B}_q(D,\mu_j,\mu_{j+1}) = \frac{1}{[(\mu_j-\mu_{j+1})!]^q}\frac{(2\alpha_j+2\mu_{j+1}+1)^q_{2(\mu_j-\mu_{j+1})}}{(2\alpha_j+\mu_j+\mu_{j+1})^q_{\mu_j-\mu_{j+1}}}\frac{(q\mu_{j+1}+\alpha_j+1)_{q(\mu_j-\mu_{j+1})}}{(\alpha_j+\mu_{j+1}+1)^q_{\mu_j-\mu_{j+1}}} \tag{78}$$

and

$$\begin{aligned} \mathcal{G}_q(D,\mu_j,\mu_{j+1}) &= F^{1:2;\ldots;2}_{1:1;\ldots;1}\left(\begin{array}{c} a_j : b_j, c_j; \ldots; b_j, c_j \\ d_j : e_j; \ldots; e_j \end{array};1,\ldots,1\right) \\ &= \sum_{i_1,\ldots,i_{2q}=0}^{\mu_j-\mu_{j+1}}\frac{(a_j)_{i_1+\ldots i_{2q}}}{(d_j)_{i_1+\ldots+i_{2q}}}\frac{(b_j)_{i_1}(c_j)_{i_1}\cdots(b_j)_{i_{2q}}(c_j)_{i_{2q}}}{(e_j)_{i_1}\cdots(e_j)_{i_{2q}}i_1!\cdots i_{2q}!} \end{aligned} \tag{79}$$

with $a_j = \alpha_j + q\mu_{j+1} + \frac{1}{2}$, $b_j = -\mu_j + \mu_{j+1}$, $c_j = 2\alpha_j + \mu_{j+1} + \mu_j$, $d_j = 2q\mu_{j+1} + 2\alpha_j + 1$ and $e_j = \alpha_j + \mu_{j+1} + \frac{1}{2}$, respectively. Note that the sum becomes finite because b_j is a negative integer number, and so the Pochhammer numbers $(b_j)_i = \frac{\Gamma(b_j+i)}{\Gamma(b_j)} = 0, \quad \forall i > |b_j|$. Let us also highlight that when $\mu_j = \mu_{j+1}$, the function $\mathcal{B}_q(D, \mu_j, \mu_{j+1}) = \mathcal{G}_q(D, \mu_j, \mu_{j+1}) = 1$.

Moreover, the application of the previously mentioned linearization techniques to the Gegenbauer functionals of (72) and (74) together with Equation (68) allowed us to find [56,121] the momentum Rényi entropies of the D-dimensional hydrogenic states $(n, l, \{\mu\})$ as

$$\begin{aligned} R_q[\gamma_{n,l,\{\mu\}}] &= D\ln\left(\frac{\pi^{\frac{1}{2}}Z}{\eta}\right) + \frac{q}{1-q}\ln[2\eta\,(\eta-L)_{2L+1}] \\ &+\frac{1}{1-q}\ln\left[\overline{\mathcal{F}}_q(D,\eta,L)\overline{\mathcal{A}}_q(D,L)\frac{\Gamma(l+\frac{D}{2})^q}{\Gamma\left(ql+\frac{D}{2}\right)}\frac{\Gamma(qm+1)}{\Gamma(m+1)^q}\right] \\ &+\frac{1}{1-q}\sum_{j=1}^{D-2}\ln\left[\mathcal{B}_q(D,\mu_j,\mu_{j+1})\,\mathcal{G}_q(D,\mu_j,\mu_{j+1})\right] + \ln 2 \end{aligned} \tag{80}$$

with the coefficients

$$\overline{\mathcal{A}}_q(D,L) \equiv 2^{2q-1}\frac{\Gamma\left(\frac{D}{2}+ql\right)\Gamma\left(-\frac{D}{2}+q(D+l+1)\right)}{\Gamma\left(\frac{D}{2}+l\right)^{2q}\Gamma(q(D+2l+1))} \tag{81}$$

and

$$\begin{aligned} \overline{\mathcal{F}}_q(D,\eta,L) &\equiv F^{1:2;\ldots;2}_{1:1;\ldots;1}\left(\begin{matrix} a:b,c;\ldots;b,c \\ \\ d:e;\ldots;e \end{matrix}\;;1,\ldots,1\right) \\ &= \sum_{i_1,\ldots,i_{2q}=0}^{n-l-1}\frac{(a)_{i_1+\ldots i_{2q}}}{(d)_{i_1+\ldots+i_{2q}}}\frac{(b)_{i_1}(c)_{i_1}\cdots(b)_{i_{2q}}(c)_{i_{2q}}}{(e)_{i_1}\cdots(e)_{i_{2q}}i_1!\cdots i_{2q}!}, \end{aligned} \tag{82}$$

which is a multivariate Srivastava–Daoust function [55,58] with $a = (L+\frac{3}{2})q + \frac{D}{2}(1-q)$, $b = -(\eta - L - 1)$, $c = \eta + L + 1$, $d = q(2L+4)$, $e = L + \frac{3}{2}$. The other two coefficients $\mathcal{B}_q$ and $\mathcal{G}_q$ are already given by Equations (78) and (79). Note that when $l = n-1$, the function $\mathcal{F}_q(D, \eta, L) = 1$.

Finally, the combination of Equations (63) and (75), and Equations (64) and (80) gives rise to the final expressions of the LMC–Rényi complexity measures in position and momentum spaces, respectively, for arbitrary D-dimensional hydrogenic states. These general expressions depend only on the state's hyperquantum numbers $(n, l, \{\mu\})$, the nuclear charge Z and the space dimensionality D. They are, however, somewhat highbrow but allow to determine the values of the Rényi complexity measures by general-purpose symbolic-like computer program systems (see [108,109]) in an algorithmic way. For low values of the involved parameters (α, β), the corresponding complexity-like measures are analytically obtained in a compact manner for some particular hydrogenic states, such as the quasi-spherical and ground states. The relevant case ($\alpha \to 1, \beta = 2$) of the LMC–Rényi complexity (3), which corresponds to the pioneering LMC (López-Ruiz–Mancini–Calvet) complexity measure [15,39,40] $C_{1,2}[\rho] = \mathcal{D}[\rho] \times e^{S[\rho]}$ with $\mathcal{D}[\rho] = e^{-R_2[\rho]}$ was monographically analyzed [29] for general and quasi-spherical states in the two reciprocal spaces.

6.1. Application to Quasi-Spherical and Ground States

The application of the previous general result to the quasi-spherical states, $(n, n-1, \{n-1\}) \equiv (n, \mu_1 = \mu_2 \ldots = \mu_{D-1} = n-1)$, of the D-dimensional hydrogenic system with nuclear charge Z allowed us to find [56] the values

$$R_q[\rho_{n,n-1}] = D \ln \frac{\eta}{2Z} - \frac{q}{1-q} \ln[\Gamma(2\eta+1)] + \frac{1}{1-q} \ln\left(\frac{\Gamma(D+2nq-2q)}{q^{D+2nq-2q}}\right), \tag{83}$$

$$\begin{aligned} R_q[\gamma_{n,n-1}] &= D \ln \frac{Z}{\eta} + \frac{q}{1-q} \ln[4\,\Gamma(2\eta+1)] \\ &+ \frac{1}{1-q} \ln\left[\frac{\Gamma\left(\frac{D}{2}+qn-q\right)\Gamma\left(-\frac{D}{2}+q(D+n)\right)}{2\Gamma\left(n+\frac{D}{2}-1\right)^{2q}\Gamma(q(D+2n-1))}\right], \end{aligned} \tag{84}$$

and

$$R_q[\mathcal{Y}_{l,\{l\}}] = \ln(2\pi^{\frac{D}{2}}) + \frac{1}{1-q} \ln\left[\frac{\Gamma(l+\frac{D}{2})^q}{\Gamma(l+1)^q} \frac{\Gamma(ql+1)}{\Gamma\left(ql+\frac{D}{2}\right)}\right] \tag{85}$$

for the radial and angular Rényi entropies of the quasi-spherical states in the two reciprocal spaces, respectively. Moreover, for the case $(n = 1, l = 0, \{0\})$, these three expressions provide us with the following values:

$$R_q[\rho_{1,0}] = \Gamma(D) + D \ln\left[\frac{D-1}{4Z\, q^{\frac{1}{1-q}}}\right] \tag{86}$$

$$\begin{aligned} R_q[\gamma_{1,0}] &= D \ln\left[\frac{2Z}{D-1}\right] + \frac{q}{1-q} \ln[4\,\Gamma(D)] \\ &+ \frac{1}{1-q} \ln\left[\frac{\Gamma\left(\frac{D}{2}\right)^{1-2q}\Gamma\left(D(q-\frac{1}{2})+q\right)}{2\Gamma(Dq+q)}\right] \end{aligned} \tag{87}$$

and

$$R_q[\mathcal{Y}_{0,\{0\}}] = \ln\left[\frac{2\,\pi^{\frac{D}{2}}}{\Gamma\left(\frac{D}{2}\right)}\right] \tag{88}$$

for the radial and angular position and momentum Rényi entropies of the ground state of the D-dimensional hydrogenic system, respectively.

The corresponding position and momentum LMC-Rényi complexity measures for these quasi-spherical and ground states are given by Equations (63), (64) and (66), (68) together with the Rényi entropy values (83)–(85) and (86)–(88), respectively. A numerical study of these complexity measures was performed in [56] for a few specific three-dimensional hydrogenic states, where it is also shown that the hydrogenic Rényi entropy sum, $R_\alpha[\rho_{n,l,\{\mu\}}] + R_\beta[\gamma_{n,l,\{\mu\}}]$, fulfills the Rényi-entropy-based uncertainty relation [82,83] given by

$$R_\alpha[\rho] + R_\beta[\gamma] \geq D \log\left(2(2\beta)^{\frac{1}{2-2\beta}}(2\alpha)^{\frac{1}{2-2\alpha}}\right), \quad \frac{1}{\alpha} + \frac{1}{\beta} = 2, \tag{89}$$

which is universally valid.

6.2. Application to Highly Excited Rydberg States

According to (63) and (66), the LMC–Rényi complexity measures of the highly excited Rydberg states (i.e., states $(n,l,\{\mu\})$ with $n\to\infty; l,m$ fixed) are given by

$$\overline{C}^{(Ry)}_{\alpha,\beta}[\rho_{n,l,\{\mu\}}] := e^{\frac{1}{D}(R^{(Ry)}_{\alpha}[\rho_{n,l,\{\mu\}}]-R^{(Ry)}_{\beta}[\rho_{n,l,\{\mu\}}])}, \quad 0<\alpha<\beta<\infty, \quad \alpha,\beta\neq 1, \tag{90}$$

and

$$\overline{C}^{(Ry)}_{\alpha',\beta'}[\gamma_{n,l,\{\mu\}}] := e^{\frac{1}{D}(R^{(Ry)}_{\alpha'}[\rho_{n,l,\{\mu\}}]-R^{(Ry)}_{\beta'}[\gamma_{n,l,\{\mu\}}])}, \quad 0<\alpha'<\beta'<\infty, \quad \alpha',\beta'\neq 1, \tag{91}$$

in the position and momentum spaces, respectively. The symbols $R^{(Ry)}_q[\rho_{n,l,\{\mu\}}]$ and $R^{(Ry)}_q[\gamma_{n,l,\{\mu\}}]$ (with natural q other than unity) denote the position and momentum Rényi entropies (65) of the D-dimensional Rydberg hydrogenic states, respectively. According to (66) and (70), the position Rényi entropies (65) of the D-dimensional Rydberg hydrogenic states are given by

$$\begin{aligned} R^{(Ry)}_q[\rho_{n,l,\{\mu\}}] &\simeq \frac{1}{1-q}\log N_\infty(n,l,D,q) + R_q[\mathcal{Y}_{l,\{\mu\}}] \\ &+ D\log\frac{\eta}{2Z} - \frac{q}{1-q}\log(2\eta) &(92)\\ &\simeq \frac{1}{1-q}\log N_\infty(n,l,D,q) + D\log\frac{n}{2Z} - \frac{q}{1-q}\log(2n) &(93)\end{aligned}$$

with

$$N_\infty(n,l,D,q) = \lim_{n\to\infty}\int_0^\infty\left(\left[\tilde{\mathcal{L}}^{(\alpha)}_n(x)\right]^2 w_\alpha(x)\right)^q x^\beta\,dx \tag{94}$$

with $\alpha = 2l+D-2$ and $\beta = (2-D)q+D-1$. Now, taking into account the strong asymptotics of Laguerre polynomials [115,117] (see [112] for further details) we have obtained for $D>2$ that

$$N_\infty(n,l,D,q) = c(\beta,q)\,(2(n-l-1))^{1+\beta-q}\,(1+\bar{o}(1)), \tag{95}$$

for $q\in\left(0,\frac{D-1}{D-2}\right)$ and the constant

$$c(\beta,q) := \frac{2^{\beta+1}}{\pi^{q+1/2}}\,\frac{\Gamma(\beta+1-q/2)\,\Gamma(1-q/2)\,\Gamma(q+1/2)}{\Gamma(\beta+2-q)\,\Gamma(1+q)}. \tag{96}$$

Let us highlight that the position Rényi entropies of three-dimensional hydrogenic system was monographically studied analytically and numerically [111]. For the remaining pairs (D,q), the asymptotical value $N_\infty(n,l,D,q)$ has also been found [112].

Similarly, according to (68) and (72), the momentum Rényi entropies (67) of the D-dimensional Rydberg hydrogenic states are given by

$$\begin{aligned} R^{(Ry)}_q[\gamma_{n,l,\{\mu\}}] &\simeq \frac{1}{1-q}\log I_\infty(n,l,q,D) + R_q[\mathcal{Y}_{l,\{\mu\}}] + D\log\frac{Z}{\eta}, &(97)\\ &\simeq \frac{1}{1-q}\log I_\infty(n,l,q,D) + D\log\frac{Z}{n}, &(98)\end{aligned}$$

with

$$I_\infty(n,l,q,D) = \lim_{n\to\infty}\int_{-1}^{1}\left\{[\tilde{C}^{(l+\frac{D-1}{2})}_{n-l-1}(y)]^2\,\omega_{l+\frac{D-1}{2}}(y)\right\}^q(1-y)^a(1+y)^b\,dy, \tag{99}$$

which was recently calculated [113] at first order. One finally has that

$$R_q^{(Ry)}[\gamma_{n,l,\{\mu\}}] \begin{cases} \sim -\frac{3q}{1-q}\log n\,, & q \in (q_*, q^*) \\ = -D\log n + \frac{1}{1-q}\log\log n + O(1), & q = q^* \\ = -D\log n + \frac{1}{1-q}\log c'(q,D) + o(1)\,, & q \in (q^*, q^+) \\ = -D\log n + \frac{1}{1-q}\log\log n + O(1), & q = q^+ \\ \asymp (-2D - \frac{q}{1-q})\log n\,, & q > q^+ \end{cases} \tag{100}$$

for $n >> 1$, $l = 0,1,2,\ldots$ and $D > 0$. The symbols $q_* := \frac{1}{2}\frac{D}{l+D+1}$, $q^* := \frac{D}{D+3}$ and $q^+ := \frac{D}{D-1}$. Moreover, $q_* = q^*$ for $D = 1$ and $l = 0$, and $q_* < q^*$ for $D > 1$; the constant $c'(q,D)$ has the value

$$c'(q,D) = \frac{2^{a+b+1}}{\pi^{q+1}}\frac{\Gamma(q+\frac{1}{2})\Gamma(\frac{1}{2})}{\Gamma(q+1)}\frac{\Gamma(a-\frac{q}{2}+1)\Gamma(b-\frac{q}{2}+1)}{\Gamma(a+b-q+2)}.$$

So that the momentum Rényi entropies of Rydberg hydrogenic states grow logarithmically with n for all $q > q_*$. Finally, it is interesting to realize from Equations (93)–(95) and (100) that the net sum of Rényi entropies $R_q^{(Ry)}[\rho_{n,l,\{\mu\}}] + R_p^{(Ry)}[\gamma_{n,l,\{\mu\}}]$ of the Rydberg hydrogenic states does not depend on the nuclear charge Z of the system (as expected [101]) and verifies not only the universal Rényi entropy uncertainty relation for D-dimensional quantum systems [82,83] given by

$$R_{q_1}[\rho_{\{n_i\}}] + R_{q_2}[\gamma_{\{n_i\}}] \geq D\log\left(\pi q_1^{\frac{1}{2q_1-2}} q_2^{\frac{1}{2q_2-2}}\right)$$

with the conjugated parameters q_1 and q_2, but also the (conjectured) Rényi entropy uncertainty relation for D-dimensional quantum systems subject to a central potential [123].

7. Concluding Remarks

The multidimensional hydrogenic system encompasses numerous standard and non-standard quantum objects, ranging from the three-dimensional hydrogenic atoms to the low-dimensional semiconductor excitons and the high-dimensional qubits and Rydberg systems. In this work, we determine and review the main monotone complexity-like statistical measures [7] of this system, inspired by the theory of the quantum information of fermionic systems to a great extent; namely, the Crámer–Rao, Fisher–Shannon and LMC–Rényi measures.

These three complexity-like measures, each describing jointly two macroscopic spreading facets of the internal electronic disorder of the system, are shown to be analytically determined in terms of the state's hyperquantum numbers together with the nuclear charge and the space dimensionality. Basically, this is possible because the entropic components of these measures can be obtained in a simple (Fisher information) or a compact, although somewhat highbrow at times, manner (Shannon and Rényi entropies) manner. Keep in mind that the Fisher information has a close similarity to the multidimensional kinetic energy due to its gradient-functional form; the Shannon and Rényi entropies can be expressed by means of some logarithmic and power-like integral functionals of the Laguerre and Gegenbauer orthogonal polynomials, respectively, whose analytical evaluation is a formidable task as illustrated in [56,103], respectively.

Then, the resulting general expressions and the strong (degree) asymptotics of the Laguerre and Gegenbauer functionals are applied to evaluate the Crámer–Rao, Fisher–Shannon and LMC–Rényi complexity-like measures of the quasi-spherical and the highly excited Rydberg states of the multidimensional hydrogenic system.

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