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One-Parameter Fisher–Rényi Complexity: Notion and Hydrogenic Applications

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Abstract: In this work, the one-parameter Fisher–Rényi measure of complexity for general d-dimensional probability distributions is introduced and its main analytic properties are discussed. Then, this quantity is determined for the hydrogenic systems in terms of the quantum numbers of the quantum states and the nuclear charge.

Keywords: information theory; Fisher information; Shannon entropy; Rényi entropy; Fisher–Rényi complexity; hydrogenic systems

1. Introduction

We all have an intuitive sense of what *complexity* means. In the last two decades, an increasing number of efforts have been published [1–12] to refine our intuitions about complexity into precise, scientific concepts, pointing out a large amount of open problems. Nevertheless, there is neither a consensus on the term *complexity* nor whether there is a simple core to *complexity*. Contrary to the Boltzmann–Shannon entropy, which is ever increasing according to the second law of thermodynamics, the complexity seems to behave very differently. Various precise, widely applicable, numerical and analytical proposals (see e.g., [13–30] and the monograph [8]) have been done, but they are yet very far to appropriately formalize the intuitive notion of complexity [11,29]. The latter suggests that complexity should be minimal at either end of the scale. However, a complexity quantifier to take into account the completely ordered and completely disordered limits (i.e., perfect order and maximal randomness, respectively) and to describe/explain the maximum between them is not known up until now.

Recently, keeping in mind the fundamental principles of the density functional theory, some statistical measures of complexity have been proposed to quantify the degree of structure or pattern of finite many-particle systems in terms of their single-particle density, such as the Crámer–Rao [23,26], Fisher–Shannon [18,21,24] and LMC (López-ruiz, Mancini and Calvet) [12,17] complexities and some modifications of them [13,22,25,27–29]. They are composed by a two-factor product of entropic measures of Shannon [31], Fisher [6,32] and Rényi [33] types. Most interesting for quantum systems are those which involve the Fisher information (namely, the Crámer–Rao and the Fisher–Shannon complexities, and their modifications [25,27,34]), mainly because this is by far the best entropy-like quantity to take into account the inherent fluctuations of the quantum wave functions by quantifying the gradient content of the single-particle density of the systems.

The objective of this article is to extend and generalize these Fisher-information-based measures of complexity by introducing a new complexity quantifier, the one-parameter Fisher–Rényi complexity, to discuss its properties and to apply it to the main prototype of Coulombian systems, the hydrogenic system. This notion is composed by two factors: a λ-dependent Fisher information (which quantifies various aspects of the quantum fluctuations of the physical wave functions beyond the density gradient, since it reduces to the standard Fisher information for $\lambda = 1$) and the Rényi entropy of order λ (which measures various facets of the spreading or spatial extension of the density beyond the celebrated Shannon entropy, which corresponds to the limiting case $\lambda \to 1$).

The article is structured as follows. In Section 1, we introduce the notion of one-parameter Fisher–Rényi measure of complexity. In Section 2, we discuss the main analytical properties of this complexity, showing that it is bounded from below, invariant under scaling transformations and monotone. In addition, the near-continuity and the invariance under replications are also discussed. In Section 3, we apply the new complexity measure to the hydrogenic systems. Finally, some concluding remarks are given.

2. One-Parameter Fisher–Rényi Complexity Measure

In this section, the notion of one-parameter Fisher–Rényi complexity $C^{(\lambda)}_{FR}[\rho]$ of a d-dimensional probability density is introduced, and its main analytic properties are discussed. This quantity is composed of two entropy-like factors of local (the one-parameter Fisher information of Johnson and Vignat [35], $\tilde{F}_\lambda[\rho]$) and global (the λ-order Rényi entropy power [36], $N_\lambda[\rho]$) characters.

2.1. The Notion

The one-parameter Fisher–Rényi complexity measure $C^{(\lambda)}_{FR}[\rho]$ of the probability density $\rho(x)$, $x = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$, is defined by

$$C^{(\lambda)}_{FR}[\rho] = D_\lambda^{-1}\tilde{F}_\lambda[\rho]N_\lambda[\rho], \quad \lambda > \max\left\{\frac{d-1}{d}, \frac{d}{d+2}\right\}, \tag{1}$$

where D_λ is the normalization factor given as

$$D_\lambda = \begin{cases} 2\pi d^{\frac{\lambda-1}{\lambda-1}} \left(\frac{\Gamma\left(\frac{\lambda}{\lambda-1}\right)}{\Gamma\left(\frac{d}{2}+\frac{\lambda}{\lambda-1}\right)}\right)^{\frac{2}{d}} \left(\frac{(d+2)\lambda-d}{2\lambda}\right)^{\frac{2+d(\lambda-1)}{d(\lambda-1)}}, & \lambda > 1 \\ 2\pi d^{\frac{\lambda-1}{1-\lambda}} \left(\frac{\Gamma\left(\frac{1}{1-\lambda}-\frac{d}{2}\right)}{\Gamma\left(\frac{1}{1-\lambda}\right)}\right)^{\frac{2}{d}} \left(\frac{(d+2)\lambda-d}{2\lambda}\right)^{\frac{2+d(\lambda-1)}{d(\lambda-1)}}, & \max\left\{\frac{d-1}{d}, \frac{d}{d+2}\right\} < \lambda < 1. \end{cases} \tag{2}$$

This purely numerical factor is necessary to let the minimal value of the complexity be equal to unity, as explained below in Section 2.2.1. The $\tilde{F}_\lambda[\rho]$ denotes the (scarcely known) λ-weighted Fisher information [35] defined by

$$\tilde{F}_\lambda[\rho] = \left(\int_{\mathbb{R}^d} \rho^\lambda(x)\, dx\right)^{-1} \int_{\mathbb{R}^d} |\rho^{\lambda-2}(x)\nabla\rho(x)|^2 \rho(x)\, dx, \tag{3}$$

(which, for $\lambda = 1$, reduces to the standard Fisher information $F[\rho] = \int_{\mathbb{R}^d} \frac{|\nabla\rho|^2}{\rho}\, dx$), dx being the d-dimensional volume element. Finally, the symbol $N_\lambda[\rho]$ denotes the λ-Rényi entropy power (see e.g., [36]) given as

$$N_\lambda[\rho] = \begin{cases} \left(\int_{\mathbb{R}^d} \rho^\lambda(x)\, dx\right)^{\frac{\mu}{d}\frac{1}{1-\lambda}} & \text{if} \quad \lambda \neq 1, 0 < \lambda < \infty, \\ e^{\frac{2}{d}S[\rho]} & \text{if} \quad \lambda = 1, \end{cases} \tag{4}$$

where $\mu = 2 + d(\lambda - 1)$ and $S[\rho] := -\int_{\mathbb{R}^d} \rho(x) \ln \rho(x)\, dx$ is the Shannon entropy [31].

The complexity measure $C_{FR}^{(\lambda)}[\rho]$ has a number of conceptual advantages with respect to the Fisher-information-based measures of complexity previously defined; namely, the Crámer–Rao and Fisher–Shannon complexity and their modifications. Indeed, it quantifies the combined balance of different (λ-dependent) aspects of both the fluctuations and the spreading or spatial extension of the single-particle density ρ, in such a way that there is no dependence on any specific point of the system's region. The Crámer–Rao complexity [23,26] (which is the product of the standard Fisher information $F[\rho]$ mentioned above and the variance $V[\rho] = \langle r^2 \rangle - \langle r \rangle^2)$ measures a single aspect of the fluctuations (namely, the density gradient) together with the concentration of the probability density around the centroid $\langle r \rangle$. The Fisher–Shannon complexity [18,21,24], defined by $C_{FS}[\rho] = F[\rho] \times e^{\frac{2}{d} S[\rho]}$, quantifies the density gradient jointly with a single aspect of the spreading given by the Shannon entropy $S[\rho]$ mentioned above. A modification of the previous measure by use of the Rényi entropy $R_\lambda[\rho] = \frac{1}{1-d} \ln \int_{\mathbb{R}^d} \rho^\lambda(x)\, dx$ instead of the Shannon entropy, the Fisher–Rényi product of complexity-type, has been recently introduced [25,27,34]; it measures the gradient together with various aspects of the spreading of the density.

2.2. The Properties

Let us now discuss some properties of this notion: bounding from below, invariance under scaling transformations, monotonicity, behavior under replications and near continuity.

2.2.1. Lower Bound

The Fisher–Rényi complexity measure $C_{FR}^{(\lambda)}[\rho]$ fulfills the inequality

$$C_{FR}^{(\lambda)}[\rho] \geq 1 \tag{5}$$

(for $\lambda > \max\left\{\frac{d-1}{d}, \frac{d}{d+2}\right\}$, with $\lambda \neq 1$), and the minimal complexity occurs, as implicitly proved by Savaré and Toscani [36], if and only if the density has the following generalized Gaussian form

$$\mathcal{B}_\lambda(x) = \begin{cases} (C_\lambda - |x|^2)_+^{\frac{1}{\lambda-1}}, & \lambda > 1, \\ (C_\lambda + |x|^2)^{\frac{1}{\lambda-1}}, & \lambda < 1, \end{cases} \tag{6}$$

where $(x)_+ = \max\{x, 0\}$ and C_λ is the normalization constant given by

$$C_\lambda = A_\lambda^{-\frac{2(\lambda-1)}{d(\lambda-1)+2}}, \tag{7}$$

with

$$A_\lambda = \begin{cases} \pi^{d/2} \dfrac{\Gamma\left(\frac{\lambda}{\lambda-1}\right)}{\Gamma\left(\frac{d}{2} + \frac{\lambda}{\lambda-1}\right)}, & \lambda > 1, \\ \pi^{d/2} \dfrac{\Gamma\left(\frac{1}{1-\lambda} - \frac{d}{2}\right)}{\Gamma\left(\frac{1}{1-\lambda}\right)}, & \frac{d}{d+2} < \lambda < 1. \end{cases}$$

Thus, the complexity measure $C_{FR}^{(\lambda)}(\rho)$ has a universal lower bound of minimal complexity, which is achieved for the family of densities $\mathcal{B}_\lambda(x)$.

2.2.2. Invariance under Scaling and Translation Transformations

The complexity measure $C_{FR}^{(\lambda)}(\rho)$ is scaling and translation invariant in the sense that

$$C_{FR}^{(\lambda)}[\rho_{a,b}] = C_{FR}^{(\lambda)}[\rho], \quad \forall \lambda, \tag{8}$$

where $\rho_{a,b}(x) = a^d \rho(a(x-b))$, with $a \in \mathbb{R}$ and $b \in \mathbb{R}^d$. To prove this property, we follow the lines of Savaré and Toscani [36]. First, we calculate the generalized Fisher information of the transformed density, obtaining

$$\begin{aligned}
\tilde{F}_\lambda[\rho_{a,b}] &= \left(\int_{\mathbb{R}^d} a^{d\lambda}\rho^\lambda(a(x-b))\,dx\right)^{-1} \\
&\times \int_{\mathbb{R}^d} a^{2d(\lambda-2)}\rho^{2(\lambda-2)}(a(x-b))|a^{d+1}[\nabla\rho](a(x-b))|^2 a^d\rho(a(x-b))\,dx \\
&= a^{d(\lambda-1)+2}\left(\int_{\mathbb{R}^d}\rho^\lambda(y)\,dy\right)^{-1}\int_{\mathbb{R}^d}\rho^{2\lambda-4}(y)|\nabla\rho(y)|^2\rho(y)\,dy \\
&\equiv a^{d(\lambda-1)+2}\tilde{F}_\lambda[\rho], \quad \forall\lambda.
\end{aligned}$$

Note that, in writing the first equality, we have used

$$|\nabla\rho_{a,b}(x)|^2 = |a^{d+1}[\nabla\rho](a(x-b))|^2.$$

Then, we determine the value of the λ-entropy power of the density $\rho_{a,b}(x)$, which turns out to be equal to

$$\begin{aligned}
N_\lambda[\rho_{a,b}] &= \left(\int_{\mathbb{R}^d} a^{d\lambda}\rho^\lambda(a(x-b))\,dx\right)^{\frac{2+d(\lambda-1)}{d(1-\lambda)}} \\
&= \left(a^{d(\lambda-1)}\int_{\mathbb{R}^d}\rho^\lambda(y)\,dy\right)^{\frac{2+d(\lambda-1)}{d(1-\lambda)}} \\
&\equiv a^{-d(\lambda-1)-2}N_\lambda[\rho], \quad \forall\lambda.
\end{aligned}$$

In particular, we have

$$\begin{aligned}
N_1[\rho_{a,b}] &= \exp\left[-\frac{2}{d}\int_{\mathbb{R}^d} a^d\rho^\lambda(a(x-b))\ln[a^d\rho^\lambda(a(x-b))]\,dx\right] \\
&= \exp\left[-\frac{2}{d}\int_{\mathbb{R}^d}\rho(y)\ln[a^d\rho(y)]\,dy\right] \\
&= \exp\left[-\frac{2}{d}\left(d\ln a + S[\rho]\right)\right] \\
&\equiv a^{-2}N_1[\rho].
\end{aligned}$$

Finally, from Equation (1) and the values of $\tilde{F}_\lambda[\rho_{a,b}]$ and $N_\lambda[\rho_{a,b}]$ just found, we readily obtain the wanted invariance (8).

2.2.3. Monotonicity

The existence of a non-trivial operation with interesting properties under which a complexity measure is monotone [11] is a valuable property of the measure in question from the axiomatic point of view. To show the monotone behavior of the Fisher–Rényi complexity $C^{(\lambda)}_{FR}(\rho)$, we make use of the so-called *rearrangements*, which represent a useful tool in the theory of functional analysis, and, among other applications, have been used to prove relevant inequalities such as Young's inequality with sharp constant.

Two of the main properties of rearrangements is that they preserve the L^p norms, which implies that the rearrangements of a probability density give rise to another probability density, and that they make everything spherically symmetric. The second feature makes the rearrangement operation relevant for quantification of statistical complexity [11], since a spherically symmetric variant of a probability density can in an atomic context be viewed as less complex. Then, we introduce the definition of this operation as well as its effects over the entropic quantities that make up our complexity measure. Let f be a real-valued function, $f : \mathbb{R}^n \to [0, \infty)$ and $A_t = \{x : f(x) \geq t\}$. The symmetric decreasing rearrangement of f is defined as

$$f^*(x) = \int_0^\infty \chi_{\{x \in A_t^*\}}\, dt\,, \tag{9}$$

with $\chi_{\{x \in A_t^*\}} = 1$ if $x \in A_t^*$ and 0, otherwise. A_t represents the super-level set of the function f, and A^* (which denotes the symmetric rearrangement of a set $A \subset \mathbb{R}^n$) is the Euclidean ball centered at 0 such as $Vol(A^*) = Vol(A)$.

The central idea of this transformation is to build up f^* from the rearranged super-level sets in the same manner that f is built from its super-level sets. As a by-product from its construction, f^* turns out to be a *spherically symmetric decreasing* function (i.e., $f^*(x) = f^*(|x|)$ and moreover $f^*(b) < f^*(a)\ \forall b > a$, where $a, b \in A_t^*$), which means that, for any function $f : \mathbb{R}^n \to [0, \infty)$ and all $t \geq 0$

$$\{x : f(x) > t\}^* = \{x : f^*(x) > t\}, \tag{10}$$

or, in other words, for any measurable subset $B \subset [0, \infty)$, the volume of the sets $\{x : f(x) \in B\}$ and $\{x : f^*(x) \in B\}$ are the same.

It is known [37] that under this transformation and for any $p \in [0, 1) \cup (1, \infty]$ the Rényi and Shannon entropies remain unchanged, i.e.,

$$R_p[\rho] = R_p[\rho^*], \quad S[\rho] = S[\rho^*] \tag{11}$$

if both $S[\rho]$ and $S[\rho^*]$ are well defined, where $\lim_{p \to 1} R_p[\rho] = S[\rho]$. The invariance of the Rényi entropy follows from the preservation of the L^p norms via rearrangements and the proof of the invariance of the Shannon entropy is done in [37]. Moreover, Wang and Madiman [37] consider the Fisher information, finding that the standard Fisher information decreases monotonically under rearrangements, i.e.,

$$F[\rho] \geq F[\rho^*]. \tag{12}$$

Let us now consider the biparametric Fisher-like information, $I_{\beta,q}[f]$, of a probability density function $f(x)$, which is defined [38] by

$$I_{\beta,q}[f] = \int_{\mathbb{R}^d} f^{\beta(q-1)+1}(x) \left(\frac{|\nabla f(x)|}{f(x)}\right)^\beta f(x)\, dx, \tag{13}$$

with $q \geq 0$, $\beta > 1$. Then, one notes that the one-parameter Fisher information, $\tilde{F}_\lambda[\rho]$, given by (3), can be expressed in terms of the previous quantity with $\beta = 2$ and $q \equiv \lambda$ as

$$\tilde{F}_\lambda[\rho] = \frac{\int_{\mathbb{R}^d} |\rho^{\lambda-2}(x) \nabla \rho(x)|^2 \rho(x)\, dx}{\int_{\mathbb{R}^d} \rho^\lambda(x)\, dx} = \frac{I_{2,\lambda}[\rho]}{N_\lambda[\rho]^{\frac{\mu}{d}(1-\lambda)}}. \tag{14}$$

On the other hand, considering the transformation $\rho = u(x)^k$ with $k = \frac{\beta}{\beta(q-1)+1}$, the biparametric Fisher information becomes

$$I_{\beta,q} = \int_{\mathbb{R}^d} |\nabla u(x)|^\beta\, dx, \tag{15}$$

also known as the β-Dirichlet energy of $u(x)$. If $k = 2$, note that the function $u(x)$ corresponds to a quantum-mechanical wave function. By using the symmetric decreasing rearrangement to the density function ρ, the well-known Pólya–Szegö inequality states that

$$I_{\beta,q}[\rho] = \int_{\mathbb{R}^d} |\nabla u|^\beta \geq I_{\beta,q}[\rho^*] = \int_{\mathbb{R}^d} |\nabla u^*|^\beta, \tag{16}$$

which implies that the minimizer of the left side is necessarily radially symmetric and decreasing, so the extremal function belongs to the subset of radially symmetric probability densities, and is represented by the generalized Gaussian given in (6). Now, by taking into account (14) and the invariance of the Rényi entropy (and, therefore, the Rényi entropy power, $N_\lambda[\rho]$), upon rearrangements, one obtains the monotone behavior of $\tilde{F}_\lambda[\rho]$ as

$$\tilde{F}_\lambda[\rho] = \frac{I_{2,\lambda}[\rho]}{N_\lambda[\rho]^{\frac{\mu}{d}(1-\lambda)}} \geq \tilde{F}_\lambda[\rho^*] = \frac{I_{2,\lambda}[\rho^*]}{N_\lambda[\rho^*]^{\frac{\mu}{d}(1-\lambda)}}, \tag{17}$$

Finally, this observation together with (1) allows us to obtain the monotone behavior of this complexity measure $C_{FR}^{(\lambda)}(\rho)$ proved by rearrangements, i.e.,

$$C_{FR}^{(\lambda)}(\rho) \geq C_{FR}^{(\lambda)}(\rho^*), \tag{18}$$

where the inequality is saturated for the generalized Gaussian, $\rho(x) = \mathcal{B}_\lambda(x)$, which also means that the symmetric rearrangement of a generalized Gaussian gives another generalized Gaussian, i.e., rearrangements preserve this subset of radially symmetric probability densities $\mathcal{B}_\lambda^*(x) = \mathcal{B}_{\lambda'}(x)$.

2.2.4. Behavior under Replications

Here we study the behavior of the Fisher–Rényi complexity $C_{FR}^{(\lambda)}(\rho)$ under n replications. We have found that, for one-dimensional densities $\rho(x)$, $x \in \mathbb{R}$ with bounded support, this complexity measure behaves as follows:

$$C_{FR}[\tilde{\rho}] = n^2 C_{FR}[\rho], \tag{19}$$

where the density $\tilde{\rho}$ representing n replications of ρ is given by

$$\tilde{\rho}(x) = \sum_{m=1}^{n} \rho_m(x); \quad \rho_m(x) = n^{-\frac{1}{2}} \rho\left(n^{\frac{1}{2}}(x - b_m)\right),$$

where the points b_m are chosen such that the supports Λ_m of each density ρ_m are disjoints. Then, the integrals

$$\begin{aligned}\int_\Lambda |(\tilde{\rho}(x))^{\lambda-2}\tilde{\rho}'(x)|^2\tilde{\rho}(x)dx &= \sum_{m=1}^{n}\int_{\Lambda_m} |(\rho_m(x))^{\lambda-2}\rho_m'(x)|^2\rho_m(x)dx \\ &= \sum_{m=1}^{n} n^{-\lambda+1}\int_\Lambda |(\rho(y))^{\lambda-2}\rho'(y)|^2\rho(y)dy = n^{-\lambda+2}\int_\Lambda |(\rho(y))^{\lambda-2}\rho'(y)|^2\rho(y)dy,\end{aligned}$$

and

$$\int_\Lambda (\tilde{\rho}(x))^\lambda dx = \sum_{m=1}^{n}\int_{\Lambda_m}(\tilde{\rho}_m(x))^\lambda dx = \sum_{m=1}^{n} n^{-\frac{\lambda+1}{2}}\int_\Lambda (\rho(y))^\lambda dy = n^{-\frac{\lambda-1}{2}}\int_\Lambda (\rho(y))^\lambda dy,$$

where the change of variable $y = n^{\frac{1}{2}}(x - b_m)$ has been performed.

Thus, the two entropy factors (the generalized Fisher information and the Rényi entropy power) of the Fisher–Rényi measure $C_{FR}^{(\lambda)}(\rho)$ gets modified as

$$\tilde{F}_\lambda[\tilde{\rho}] = n^{\frac{3-\lambda}{2}}\tilde{F}_\lambda[\rho], \qquad N_\lambda[\tilde{\rho}] = n^{\frac{\lambda+1}{2}} N_\lambda[\rho], \tag{20}$$

so that from these two values and (1), we finally have the wanted behavior (19) of the Fisher–Rényi complexity under n replications. Although this has been proved in the one-dimensional case, similar arguments hold for general dimensional densities.

2.2.5. Near-Continuity Behavior

Here we illustrate that the Fisher–Rényi complexity is not near continuous by means of a one-dimensional counter-example. Recall first that a functional G is near continuous if for any $\epsilon > 0$, there exists $\delta > 0$, such that, if two densities ρ and $\tilde{\rho}$ are δ-neighboring (i.e., the Lebesgue measure of the points satisfying $|\rho(x) - \tilde{\rho}(x)| \geq \delta$ is zero), then $|G[\rho] - G[\tilde{\rho}]| < \epsilon$. Now, let us consider the δ-neighboring densities

$$\rho(x) = \frac{2}{\pi} \begin{cases} \sin^2(x), & -\pi \leq x \leq 0, \\ 0, & \text{elsewhere}, \end{cases}$$

and

$$\tilde{\rho}(x) = \frac{2}{\pi(1+\delta^6)} \begin{cases} \sin^2(x), & -\pi \leq x \leq 0, \\ \delta \sin^2\left(\frac{x}{\delta^5}\right), & 0 < x \leq \delta^5 \pi, \\ 0, & \text{elsewhere}. \end{cases}$$

Due to the increasing oscillatory behaviour of $\tilde{\rho}$ for $x \in (0, \delta^5 \pi)$ as δ tends to zero, the generalized Fisher information $\tilde{F}$ grows rapidly as δ decreases, while the Rényi entropy power tends to a constant value. Then, the more similar ρ and $\tilde{\rho}$ are, the more different are their values of $C_{FR}^{(\lambda)}$. Therefore, the Fisher–Rényi complexity measure is not near continuous.

3. The Hydrogenic Application

In this section, we determine the one-parameter Fisher–Rényi complexity measure $C_{FR}^{(\lambda)}$, given by (1), for the probability density of hydrogenic atoms consisting of an electron bound by the Coulomb potential, $V(r) = -\frac{Z}{r}$, where Z denotes the nuclear charge, $r \equiv |\vec{r}| = \sqrt{\sum_{i=1}^{3} x_i^2}$ and the position vector $\vec{r} = (x_1, x_2, x_3)$ is given in spherical polar coordinates as $(r, \theta, \phi) \equiv (r, \Omega)$, $\Omega \in S^2$. Atomic units are used. The hydrogenic states are well known to be characterized by the three quantum numbers $\{n, l, m\}$, with $n = 0, 1, 2, \ldots$, $l = 0, 1, \ldots, n-1$ and $m = -l, -l+1, \ldots, l$. They have the energies $E_n = -\frac{Z^2}{2n^2}$, and the corresponding quantum probability densities are given by

$$\rho_{n,l,m}(\vec{r}) = \rho_{n,l}(\tilde{r})\ \Theta_{l,m}(\theta, \phi) \tag{21}$$

where $\tilde{r} = \frac{2Z}{n} r$, and the symbols $\rho_{n,l}(\tilde{r})$ and $\Theta_{l,m}(\theta, \phi)$ are the radial and angular parts of the density, which are given by

$$\rho_{n,l}(\tilde{r}) = \frac{4Z^3}{n^4} \frac{\omega_{2l+1}(\tilde{r})}{\tilde{r}} [\widehat{L}_{n-l-1}^{(2l+1)}(\tilde{r})]^2, \tag{22}$$

and

$$\Theta_{l,m}(\theta, \phi) = |Y_{l,m}(\theta, \phi)|^2, \tag{23}$$

respectively. In addition, $\widehat{L}_n^{\alpha}(x)$ denotes the orthonormal Laguerre polynomials [39] with respect to the weight function $\omega_\alpha = x^\alpha e^{-x}$ on the interval $[0, \infty)$, and $Y_{l,m}(\theta, \phi)$ are the well-known spherical harmonics, which can be expressed in terms of the Gegenbauer polynomials, $C_n^m(x)$ via

$$Y_{l,m}(\theta, \phi) = \left(\frac{(l+\frac{1}{2})(l-|m|)![\Gamma(|m|+\frac{1}{2})]^2}{2^{1-2|m|}\pi^2(l+|m|)!} \right)^{\frac{1}{2}} e^{im\phi} (\sin\theta)^{|m|} C_{l-|m|}^{|m|+\frac{1}{2}}(\cos\theta), \tag{24}$$

where $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$. Let us now compute the complexity measure $C_{FR}^{(\lambda)}[\rho_{n,l,m}]$ of the hydrogenic probability density, which, according to (1), is given by

$$C_{FR}^{(\lambda)}[\rho_{n,l,m}] \quad = \quad D_\lambda^{-1} \tilde{F}_\lambda[\rho_{n,l,m}] N_\lambda[\rho_{n,l,m}] \equiv D_\lambda^{-1} I_1 I_2^{2\left(\frac{1}{3(1-\lambda)}-1\right)}, \tag{25}$$

where D_λ is the normalization constant given by (2) and the symbols I_1 and I_2 denote the integrals

$$I_1 = \int |\,[\rho_{n,l,m}(\vec{r})]^{\lambda-2}\; \nabla\rho_{n,l,m}(\vec{r})|^2\, \rho_{n,l,m}(\vec{r})\, d^3\vec{r} = \int [\rho_{n,l,m}(\vec{r})]^{2\lambda-3}\; |\nabla\rho_{n,l,m}(\vec{r})|^2\, d^3\vec{r}, \quad (26)$$

$$I_2 = \int [\rho_{n,l,m}(\vec{r})]^{\lambda}\; d^3\vec{r} = \int_0^\infty [\rho_{n,l}(\tilde{r})]^{\lambda}\; r^2\, dr \int_\Omega [\Theta_{l,m}(\theta,\phi)]^{\lambda}\; d\Omega, \quad (27)$$

which can be solved by following the lines indicated in Appendix A.

In the following, for simplicity and illustration purposes, we focus our attention on the computation of the complexity measure for two large, relevant classes of hydrogenic states: the (ns) and the circular $(l = m = n-1)$ states.

3.1. Generalized Fisher–Rényi Complexity of Hydrogenic (ns) States

For (ns) states one has $\Theta_{0,0}(\theta,\phi) = |Y_{0,0}(\theta,\phi)|^2 = \frac{1}{4\pi}$ so that the three angular integrals can be trivially determined, and the radial integrals simplify as

$$I_{1a}^{(rad)} = \frac{2^{4\lambda-3}Z^{6\lambda-4}}{n^{10\lambda-6}}(2\lambda-1)^{-1}\mathcal{G}(n,0,\lambda), \quad (28)$$

$$I_{1b}^{(rad)} = \frac{2^{4\lambda-3}Z^{6\lambda-4}}{n^{10\lambda-6}}(2\lambda-1)^{-1}\Phi_0\left(0,0,2(2\lambda-1),\{n-1\},\{1\};\left\{\frac{1}{2\lambda-1},1\right\}\right), \quad (29)$$

$$I_2^{(rad)}(\lambda) = \frac{2^{2\lambda-3}Z^{3(\lambda-1)}}{n^{5\lambda-3}}\lambda^{-3}\,\Phi_0\left(2,0,2\lambda,\{n-1\},\{1\};\left\{\frac{1}{\lambda},1\right\}\right), \quad (30)$$

with

$$\begin{aligned}\mathcal{G}(n,0,\lambda) &= (2\lambda-1)^{-2}\Bigg[\Phi_0\left(2,0,2(2\lambda-1),\{n-1,\dots,n-1\},\{1,\dots,1\};\left\{\frac{1}{2\lambda-1},1\right\}\right)\\ &+4\,\Phi_0\left(2,0,2(2\lambda-1),\{n-1,\dots,n-1,n-2,n-2\},\{1,\dots,1,2,2\};\left\{\frac{1}{2\lambda-1},1\right\}\right)\\ &+4\,\Phi_0\left(2,0,2(2\lambda-1),\{n-1,\dots,n-1,n-2\},\{1,\dots,1,2\};\left\{\frac{1}{2\lambda-1},1\right\}\right)\Bigg].\end{aligned} \quad (31)$$

Thus, finally, the one-parameter (λ) Fisher–Rényi complexity measure $C_{FR}^{(\lambda)}[\rho_{ns}]$ for the (ns)-like hydrogenic states is given by

$$C_{FR}^{(\lambda)}[\rho_{ns}] = D_\lambda^{-1}\frac{2^{3+\frac{2}{3(\lambda-1)}}\pi^{\frac{2}{3}}}{n^{-\frac{2}{3}\left(\frac{2}{\lambda-1}+5\right)}}\lambda^{\frac{2}{\lambda-1}+6}(2\lambda-1)^{-1}\mathcal{F}(n,0,\lambda), \quad (32)$$

where

$$\mathcal{F}(n,0,\lambda) = \Phi_0\left(2,0,2\lambda,\{n-1\},\{1\};\left\{\frac{1}{\lambda},1\right\}\right)^{2\left(\frac{1}{3(1-\lambda)}-1\right)}\mathcal{G}(n,0,\lambda). \quad (33)$$

In particular, for the ground state (i.e., when $n=1, l=m=0$), we have shown in Appendix B that

$$\mathcal{F}(1,0,\lambda) = 2^{2\left(\frac{1}{3(1-\lambda)}-1\right)}2(2\lambda-1)^{-2},$$

which allows us to find the following value

$$C_{FR}^{(\lambda)}[\rho_{1s}] = D_\lambda^{-1}4\pi^{\frac{2}{3}}\lambda^{\frac{2}{\lambda-1}+6}(2\lambda-1)^{-3} \quad (34)$$

for the one-parameter Fisher–Rényi complexity measure of the hydrogenic ground state, keeping in mind the value (2) for the normalization factor D_λ. We have done this calculation in detail to check our methodology; we are aware that, in this concrete example, it would have been simpler to start directly from the explicit expression of the wave function of the orbital 1s. Operating in a similar way, we can obtain the complexity values for the rest of the ns-orbitals.

3.2. Generalized Fisher–Rényi Complexity of Hydrogenic Circular States

For circular states the degree and parameter, $n-l-1$ and $2l+1$, of the orthonormal Laguerre polynomials, become 0 and $2n-1$, respectively, so that the corresponding polynomials simplify as $\widehat{L}_0^{(2n-1)}(\tilde{r}) = \frac{1}{\sqrt{\Gamma(2n)}}$, and then the involved radial integrals follow as

$$\begin{aligned} I_{1a}^{(rad)} &= \int_0^\infty [\rho_{n,l}(\tilde{r})]^{2\lambda-3} \left[\frac{d}{dr}\rho_{n,l}(\tilde{r})\right]^2 r^2\,dr \\ &= \frac{2^{4\lambda-3}Z^{6\lambda-4}}{n^{8\lambda-5}} \int_0^\infty \left\{[\widehat{L}_{n-l-1}^{(\alpha)}(\tilde{r})]^2\omega_\alpha(\tilde{r})\right\}^{2\lambda-3} \left\{\frac{d}{d\tilde{r}}\left([\widehat{L}_{n-l-1}^{(\alpha)}(\tilde{r})]^2\frac{\omega_\alpha(\tilde{r})}{\tilde{r}}\right)\right\}^2 \tilde{r}^{5-2\lambda}\,d\tilde{r} \\ &= \frac{2^{4\lambda-3}Z^{6\lambda-4}}{n^{8\lambda-5}} \left[\widehat{L}_0^{(2n-1)}\right]^{4\lambda-2} \int_0^\infty \omega_{2n-1}(\tilde{r})^{2\lambda-3}(\omega'_{2n-1}(\tilde{r})\tilde{r} - \omega_{2n-1}(\tilde{r}))^2\,\tilde{r}^{1-2\lambda}\,d\tilde{r} \\ &= \frac{2^{2(2\lambda-1)}Z^{2(3\lambda-2)}}{n^{8\lambda-5}}(2\lambda(n-1)-n+2)(2\lambda-1)^{4\lambda(1-n)+2n-5}\frac{\Gamma[3-2n+4\lambda(n-1)]}{[\Gamma(2n)]^{2\lambda-1}}, \end{aligned} \tag{35}$$

$$\begin{aligned} I_{1b}^{(rad)} &= \int_0^\infty [\rho_{n,l}(\tilde{r})]^{2\lambda-1}\,dr \\ &= \frac{2^{4\lambda-3}Z^{2(3\lambda-2)}}{n^{8\lambda-5}}(2\lambda-1)^{4\lambda(1-n)+2n-3}\,\frac{\Gamma[3-2n+4\lambda(n-1)]}{[\Gamma(2n)]^{2\lambda-1}}, \end{aligned} \tag{36}$$

$$\begin{aligned} I_2^{(rad)}(\lambda) &= \int_0^\infty [\rho_{n,l}(\tilde{r})]^\lambda\, r^2\,dr \\ &= \frac{2^{2\lambda-3}Z^{3(\lambda-1)}}{n^{4\lambda-3}} \int_0^\infty \left\{[\widehat{L}_{n-l-1}^{(\alpha)}(\tilde{r})]^2\omega_\alpha(\tilde{r})\right\}^\lambda \tilde{r}^{2-\lambda}\,d\tilde{r} \\ &= \frac{2^{2\lambda-3}Z^{3(\lambda-1)}}{n^{4\lambda-3}}[\widehat{L}_0^{(2n-1)}]^{2\lambda} \int_0^\infty \omega_{2n-1}(\tilde{r})^\lambda \tilde{r}^{2-\lambda}\,d\tilde{r} \\ &= \frac{2^{2\lambda-3}Z^{3(\lambda-1)}}{n^{4\lambda-3}}[\widehat{L}_0^{(2n-1)}]^{2\lambda} \int_0^\infty e^{-\lambda\tilde{r}}\tilde{r}^{2(1+\lambda(n-1))}\,d\tilde{r} \\ &= \frac{2^{2\lambda-3}Z^{3(\lambda-1)}}{n^{4\lambda-3}}\lambda^{-2\lambda(n-1)-3}\frac{\Gamma[2(n-1)\lambda+3]}{[\Gamma(2n)]^\lambda}. \end{aligned} \tag{37}$$

On the other hand, the angular part of the wavefunction for the circular states reduces as

$$\Theta_{n-1,n-1}(\theta,\phi) = |Y_{n-1,n-1}(\theta,\phi)|^2 = \frac{\Gamma(n+1/2)}{2\pi^{3/2}\Gamma(n)}(\sin\theta)^{2(n-1)}, \tag{38}$$

which allows us to readily compute the angular integrals $I_{1a}^{(ang)}$, $I_{1b}^{(ang)}$ and $I_2^{(ang)}$ as

$$\begin{aligned} I_{1a}^{(ang)} &= 2\pi\left[\frac{\Gamma(n+1/2)}{2\pi^{3/2}\Gamma(n)}\right]^{2\lambda-1}\int_0^\pi(\sin\theta)^{2(n-1)(2\lambda-1)}\sin\theta\,d\theta \\ &= 2^{2(1-\lambda)}\pi^{3(1-\lambda)}\left[\frac{\Gamma(n+1/2)}{\Gamma(n)}\right]^{2\lambda-1}\frac{\Gamma(2-n+2\lambda(n-1))}{\Gamma(5/2-n+2\lambda(n-1))}, \end{aligned} \tag{39}$$

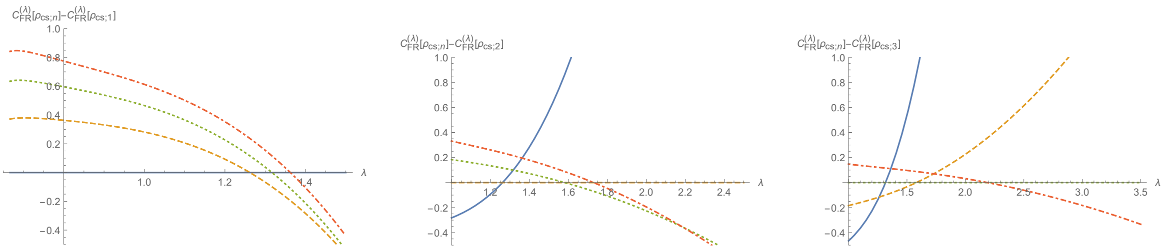
$$\begin{aligned} I_{1b}^{(ang)} &= 2\pi\left[\frac{\Gamma(n+1/2)}{2\pi^{3/2}\Gamma(n)}\right]^{2\lambda-1}\int_0^\pi(\sin\theta)^{2(n-1)(2\lambda-3)}\left[\frac{d}{d\theta}(\sin\theta)^{2(n-1)}\right]^2\sin\theta\,d\theta \\ &= 2^{3-2\lambda}\pi^{3(1-\lambda)}(n-1)^2\left[\frac{\Gamma\left(n+\frac{1}{2}\right)}{\Gamma(n)}\right]^{2\lambda-1}\frac{\Gamma[(2\lambda-1)(n-1)]}{\Gamma\left[2\lambda(n-1)-n+\frac{5}{2}\right]}, \end{aligned} \tag{40}$$

$$\begin{aligned} I_2^{(ang)} &= 2\pi\left[\frac{\Gamma(n+1/2)}{2\pi^{3/2}\Gamma(n)}\right]^\lambda\int_0^\pi(\sin\theta)^{2(n-1)\lambda}\sin\theta\,d\theta \\ &= 2^{1-\lambda}\pi^{\frac{3}{2}(1-\lambda)}\left[\frac{\Gamma(n+1/2)}{\Gamma(n)}\right]^\lambda\frac{\Gamma[1+\lambda(n-1)]}{\Gamma[\frac{3}{2}+\lambda(n-1)]}. \end{aligned} \tag{41}$$

Gathering the last six numbered expressions together with Equations (A2) and (A5), one finally obtains, according to (25), the following value

$$\begin{aligned} C_{FR}^{(\lambda)}[\rho_{cs;n}] &= D_\lambda^{-1} \frac{2^{\frac{19}{3}-4\lambda+\frac{2}{3(\lambda-1)}+n(4\lambda-2)}\pi^{\frac{1}{2}}}{n^{\frac{2}{3(1-\lambda)}-\frac{5}{3}}} \lambda^{\frac{2(3\lambda-2)(2\lambda(n-1)+3)}{3(\lambda-1)}} (2\lambda-1)^{4\lambda(1-n)+2n-5} \\ &\times \frac{[\Gamma(n)\Gamma(2n)]^{\frac{2}{3(\lambda-1)}+\frac{5}{3}}\Gamma[2-n+2\lambda(n-1)]^2}{\Gamma\left(n+\frac{1}{2}\right)^{\frac{3-5\lambda}{3(1-\lambda)}}} \left[\frac{\Gamma\left(\frac{3}{2}+\lambda(n-1)\right)}{\Gamma(1+\lambda(n-1))\Gamma(3+2\lambda(n-1))}\right]^{2\left(\frac{1}{3(\lambda-1)}+1\right)} \end{aligned} \tag{42}$$

for the one-parameter Fisher–Rényi complexity measure of the hydrogenic circular states. This expression gives for the ground state (which is also a particular circular state with $l = n - 1 = 0$) the same previously obtained value (34), which is a further checking of our results. To better understand this complicated formula, we depict in Figure 1 the behavior of the complexity measure of circular states, $C_{FR}^{(\lambda)}[\rho_{cs;n}]$, as a function of λ. This figure contains three graphs which correspond to the complexity differences $C_{FR}^{(\lambda)}[\rho_{cs;n_2}] - C_{FR}^{(\lambda)}[\rho_{cs;n_1}]$ for $n_2 = 1$ (solid blue), 2 (dashed yellow), 3 (dotted green) and 4 (dot dashed red), and with fixed $n_1 = 1$ (Figure 1a), 2 (Figure 1b) and 3 (Figure 1c).



(a) **(b)** **(c)**

Figure 1. Dependence of the complexity difference $C_{FR}^{(\lambda)}[\rho_{cs;n_2}] - C_{FR}^{(\lambda)}[\rho_{cs;n_1}]$ on λ for $n_2 = 1$ (solid blue), 2 (dashed yellow), 3 (dotted green) and 4 (dot dashed red), and with fixed $n_1 = 1$ (**a**), 2 (**b**) and 3 (**c**).

We observe that there exists a λ-dependence behavior for every couple of states (n_1, n_2) in the following sense

$$\begin{cases} C_{FR}^{(\lambda)}[\rho_{cs;n_1}] \leq C_{FR}^{(\lambda)}[\rho_{cs;n_2}], & \lambda \leq \tilde{\lambda}(n_1, n_2), \\ C_{FR}^{(\lambda)}[\rho_{cs;n_1}] \leq C_{FR}^{(\lambda)}[\rho_{cs;n_2}], & \lambda \geq \tilde{\lambda}(n_1, n_2)\,. \end{cases} \tag{43}$$

Physically, this means that for small λ (i.e., close to its lowest value), the circular states become more complex as n increases (as one can intuitively think). However, for every couple of quantum numbers (n_1, n_2), we conjecture existence of a critical value $\tilde{\lambda}(n_1, n_2)$ for which the complexity of both states is the same, while for larger values of λ, the complexity dominance becomes swapped. This phenomenon would imply that, for very large values of λ, the complexity ordering of the set of circular states becomes completely reversed. The conjectured effect shows the existence of two $\lambda-$dependent regimes of complexity and provides a novel complexity-related insight into the internal structure of the states of the system under study.

4. Conclusions

In this article, we first explored the notion of a complexity quantifier for the finite quantum many-particle systems, the one-parameter Fisher–Rényi complexity, and also examined its main analytical properties. This notion extends all the previously known measures of complexity which are sensitive to the quantum fluctuations of the physical wavefunctions of the systems (Crámer–Rao, Fisher–Shannon, Fisher–Rényi-type) in the following sense: it does not depend on any specific point of the system's region (opposite to the Crámer–Rao measure) and it quantifies the combined balance of various aspects of the fluctuations of the single-particle density beyond the gradient content (opposite to the Fisher–Shannon complexity and the Fisher–Rényi product, which only take into account a single aspect given by the density gradient content) and different facets of the spreading of this density function.

Then, we illustrated the applicability of this novel measure of complexity in the main prototype of electronic systems, the hydrogenic atom. We have obtained an analytically, algorithmic way to calculate its values for all quantum hydrogenic states, and we have given the explicit values for all the *ns* states and the circular states, which are specially relevant per se because they can be used as reference values for the complexity of Coulombian systems as reflected by the rich three-dimensional geometries of the electron density corresponding to their quantum states.

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Appendix A. Calculation of the Fisher and Rényi-like Hydrogenic Integrals

Let us here show the methodology to solve the integrals

$$I_1 = \int |\left[\rho_{n,l,m}(\vec{r})\right]^{\lambda-2} \; \nabla\rho_{n,l,m}(\vec{r})|^2 \rho_{n,l,m}(\vec{r})\, d\vec{r} = \int \left[\rho_{n,l,m}(\vec{r})\right]^{2\lambda-3} \; |\nabla\rho_{n,l,m}(\vec{r})|^2\, d\vec{r}, \tag{A1}$$

$$I_2 = \int \left[\rho_{n,l,m}(\vec{r})\right]^{\lambda} \; d\vec{r} = I_2^{(rad)} \times I_2^{(ang)}, \tag{A2}$$

with

$$I_2^{(rad)}(\lambda) = \int_0^\infty \left[\rho_{n,l}(\tilde{r})\right]^{\lambda} r^2\, dr, \tag{A3}$$

and

$$I_2^{(ang)}(\lambda) = \int_\Omega \left[\Theta_{l,m}(\theta,\phi)\right]^{\lambda} \; d\Omega \tag{A4}$$

encountered in Section 3. Since the gradient operator is $\nabla = \left(\frac{\partial}{\partial r}, \frac{1}{r}\frac{\partial}{\partial\theta}, \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\right)$ and the probability density does not depend on the azimuthal angle, ϕ, the integral I_1 can be written as

$$\begin{aligned} I_1 &= \int \left[\rho_{n,l,m}(\vec{r})\right]^{2\lambda-3} \left[\frac{\partial}{\partial r}\rho_{n,l,m}(\vec{r})\right]^2 d^3\vec{r} + \int \left[\rho_{n,l,m}(\vec{r})\right]^{2\lambda-3} \left[\frac{1}{r}\frac{\partial}{\partial\theta}\rho_{n,l,m}(\vec{r})\right]^2 d^3\vec{r} \\ &\equiv I_{1a}^{(rad)} \times I_{1a}^{(ang)} + I_{1b}^{(rad)} \times I_{1b}^{(ang)}, \end{aligned} \tag{A5}$$

where one has used $\frac{d}{dr} = \frac{2Z}{n}\frac{d}{d\tilde{r}}$, and

$$I_{1a}^{(rad)} = \int_0^\infty \left[\rho_{n,l}(\tilde{r})\right]^{2\lambda-3} \left[\frac{d}{dr}\rho_{n,l}(\tilde{r})\right]^2 r^2\, dr, \tag{A6}$$

$$I_{1b}^{(rad)} = \int_0^\infty \left[\rho_{n,l}(\tilde{r})\right]^{2\lambda-1} \; dr, \tag{A7}$$

and

$$I_{1a}^{(ang)} = \int_\Omega [\Theta_{l,m}(\theta,\phi)]^{2\lambda-1}\, d\Omega = I_2^{(ang)}(2\lambda-1), \tag{A8}$$

$$I_{1b}^{(ang)} = \int_\Omega [\Theta_{l,m}(\theta,\phi)]^{2\lambda-3}\left[\frac{d}{d\theta}\Theta_{l,m}(\theta,\phi)\right]^2 d\Omega. \tag{A9}$$

Then, the complexity measure (25) can be rewritten as

$$\begin{aligned} C_{FR}^{(\lambda)}[\rho_{n,l,m}] = {} & D_\lambda^{-1}\left[I_{1a}^{(rad)} \times \left(I_2^{(rad)}\right)^{2\left(\frac{1}{3(1-\lambda)}-1\right)}\right]\left[I_{1a}^{(ang)} \times \left(I_2^{(ang)}\right)^{2\left(\frac{1}{3(1-\lambda)}-1\right)}\right] \\ & + \left[I_{1b}^{(rad)} \times \left(I_2^{(rad)}\right)^{2\left(\frac{1}{3(1-\lambda)}-1\right)}\right]\left[I_{1b}^{(ang)} \times \left(I_2^{(ang)}\right)^{2\left(\frac{1}{3(1-\lambda)}-1\right)}\right]. \end{aligned} \tag{A10}$$

It remains to calculate the radial integrals $I_{1a}^{(rad)}$, $I_{1b}^{(rad)}$ and $I_2^{(rad)}$ and the angular integrals $I_{1a}^{(ang)}$, $I_{1b}^{(ang)}$ and $I_2^{(ang)}$. Let us start with the analytical determination of the radial integrals $I_1^{(rad)}$ and $I_2^{(rad)}$. To do this, we use the differential relation of the Laguerre polynomials [39]

$$\frac{d}{dx}L_n^{(\alpha)}(x) = -L_{n-1}^{(\alpha+1)}(x), \tag{A11}$$

and the linearization-like formula of Srivastava–Niukkanen [40,41] for the product of several Laguerre polynomials given by

$$x^\mu L_{m_1}^{(\alpha_1)}(t_1 x)\cdots L_{m_r}^{(\alpha_r)}(t_r x) = \sum_{k=0}^{\infty} \Phi_k(\mu,\beta,r,\{m_i\},\{\alpha_i\};\{t_i,1\})L_k^{(\beta)}(x), \tag{A12}$$

where the Φ_k-linearization coeffients are

$$\begin{aligned} \Phi_k(\mu,\beta,r,\{m_i\},\{\alpha_i\};\{t_i,1\}) = {} & (\beta+1)_\mu \binom{m_1+\alpha_1}{m_1}\cdots\binom{m_r+\alpha_r}{m_r}\times \\ & F_A^{r+1}(\beta+\mu+1,-m_1,\ldots,-m_r,-k;\alpha_1+1,\ldots,\alpha_r+1,\beta+1;t_1,\ldots,t_r,1), \end{aligned} \tag{A13}$$

with the Pochhammer symbol [39] $(a)_\mu$, the binomial number $\binom{a}{b}$, and the Lauricella hypergeometric function of $(r+1)$ variables F_A^{r+1} [40,41].

Then, we obtain the following analytical expressions for the radial integrals in terms of the parameters $\{Z,\lambda,n,l\}$ of the system:

$$I_{1a}^{(rad)} = \frac{2^{4\lambda-3}Z^{6\lambda-4}}{n^{8\lambda-5}}\left[\frac{\Gamma(n-l)}{\Gamma(n+l+1)}\right]^{2\lambda-1}(2\lambda-1)^{-2l(2\lambda-1)-1}\mathcal{G}(n,l,\lambda), \tag{A14}$$

$$\begin{aligned} I_{1b}^{(rad)} = {} & \frac{2^{4\lambda-3}Z^{6\lambda-4}}{n^{8\lambda-5}}\left[\frac{\Gamma(n-l)}{\Gamma(n+l+1)}\right]^{2\lambda-1}(2\lambda-1)^{-2l(2\lambda-1)-1} \\ & \times\Phi_0\left(2l(2\lambda-1),0,2(2\lambda-1),\{n-l-1\},\{2l+1\};\left\{\frac{1}{2\lambda-1},1\right\}\right), \end{aligned} \tag{A15}$$

$$\begin{aligned} I_2^{(rad)}(\lambda) = {} & \frac{2^{2\lambda-3}Z^{3(\lambda-1)}}{n^{4\lambda-3}}\left[\frac{\Gamma(n-l)}{\Gamma(n+l+1)}\right]^{\lambda}\lambda^{-2l\lambda-3} \\ & \times\Phi_0\left(2(l\lambda+1),0,2\lambda,\{n-l-1\},\{2l+1\};\left\{\frac{1}{\lambda},1\right\}\right), \end{aligned} \tag{A16}$$

where $\mathcal{G}(n,l,\lambda)$ is

$$\begin{aligned}
\mathcal{G}(n,l,\lambda) = & \Big[4l^2\Phi_0\left(2l(2\lambda-1),0,2(2\lambda-1),\{n-l-1,\ldots,n-l-1\},\{2l+1,\ldots,2l+1\};\left\{\tfrac{1}{2\lambda-1},1\right\}\right) \\
& +(2\lambda-1)^{-2} \\
& \times\Phi_0\left(2l(2\lambda-1)+2,0,2(2\lambda-1),\{n-l-1,\ldots,n-l-1\},\{2l+1,\ldots,2l+1\};\left\{\tfrac{1}{2\lambda-1},1\right\}\right) \\
& -4l(2\lambda-1)^{-1} \\
& \times\Phi_0\left(2l(2\lambda-1)+1,0,2(2\lambda-1),\{n-l-1,\ldots,n-l-1\},\{2l+1,\ldots,2l+1\};\left\{\tfrac{1}{2\lambda-1},1\right\}\right) \\
& +\tfrac{4}{(2\lambda-1)^2}\times \\
& \Phi_0\Bigg(2l(2\lambda-1)+2,0,2(2\lambda-1),\{n-l-1,\ldots,n-l-1,n-l-2,n-l-2\}, \\
& \{2l+1,\ldots,2l+1,2l+2,2l+2\};\left\{\tfrac{1}{2\lambda-1},1\right\}\Bigg) \\
& -\tfrac{8l}{(2\lambda-1)}\times \\
& \Phi_0\Bigg(2l(2\lambda-1)+1,0,2(2\lambda-1),\{n-l-1,\ldots,n-l-1,n-l-2\}, \\
& \{2l+1,\ldots,2l+1,2l+2\};\left\{\tfrac{1}{2\lambda-1},1\right\}\Bigg) \\
& +\tfrac{4}{(2\lambda-1)^2}\times \\
& \Phi_0\Bigg(2l(2\lambda-1)+2,0,2(2\lambda-1),\{n-l-1,\ldots,n-l-1,n-l-2\}, \\
& \{2l+1,\ldots,2l+1,2l+2\};\left\{\tfrac{1}{2\lambda-1},1\right\}\Bigg)\Big],
\end{aligned} \tag{A17}$$

where one should keep in mind that the Φ_0 functions are given as in (A13).

Similarly, we can obtain the angular integrals by means of linerization-like formulas of the Gegenbauer polynomials or the associated Legendre polynomials of the first kind.

Appendix B. Calculation of $\mathcal{F}(1,0,\lambda)$

Here, we will determine the value of

$$\mathcal{F}(1,0,\lambda) = \Phi_0\left(2,0,2\lambda,\{0\},\{1\};\left\{\frac{1}{\lambda},1\right\}\right)^{2\left(\frac{1}{3(1-\lambda)}-1\right)}\mathcal{G}(1,0,\lambda),$$

where

$$\begin{aligned}
\Phi_0\left(2,0,2\lambda,\{0\},\{1\};\left\{\frac{1}{\lambda},1\right\}\right) &= (1)_2\binom{1}{0}^{2\lambda}F_A^{2\lambda+1}\left(3,0,\ldots,0,0;2,\ldots,2,1;\frac{1}{\lambda},\ldots,\frac{1}{\lambda},1\right) \\
= \sum_{j_1,\ldots,j_{2\lambda+1}=0}^{\infty}\frac{(3)_{j_1+\ldots+j_{2\lambda+1}}(0)_{j_1}\ldots(0)_{j_{2\lambda+1}}}{(2)_{j_1}\ldots(2)_{j_{2\lambda+1}}}&\left(\frac{1}{\lambda}\right)^{j_1+\ldots+j_{2\lambda+1}}\frac{1}{j_1!\ldots j_{2\lambda+1}!} = 2,
\end{aligned}$$

and

$$\begin{aligned}
\mathcal{G}(1,0,\lambda) &= (2\lambda-1)^{-2}\Bigg[\Phi_0\left(2,0,2(2\lambda-1),\{0\},\{1\};\left\{\frac{1}{2\lambda-1},1\right\}\right) \\
&\quad +4\Phi_0\left(2,0,2(2\lambda-1),\{0,\ldots,0,-1,-1\},\{1,\ldots,1,2,2\};\left\{\frac{1}{2\lambda-1},1\right\}\right) \\
&\quad +4\Phi_0\left(2,0,2(2\lambda-1),\{0,\ldots,0,-1\},\{1,\ldots,1,2\};\left\{\frac{1}{2\lambda-1},1\right\}\right)\Bigg] \\
&= (2\lambda-1)^{-2}[2+4\cdot 0+4\cdot 0] = 2(2\lambda-1)^{-2},
\end{aligned}$$

since

$$\Phi_0\left(2,0,2(2\lambda-1),\{0,\dots,0,-1\},\{1,\dots,1,2\};\left\{\frac{1}{2\lambda-1},1\right\}\right)$$
$$=(1)_0\binom{1}{0}^{2(2\lambda-1)-1}\binom{1}{-1}F_A^{2(2\lambda-1)+1}(\dots)=0.$$

Then, we obtain that

$$\mathcal{F}(1,0,\lambda)=2^{2\left(\frac{1}{3(\lambda-1)}-1\right)}2(2\lambda-1)^{-2}.$$

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