

Universidad de Granada



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# Complexity and Entropic Uncertainty of Quantum Systems

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TESIS DOCTORAL

por

**David Puertas Centeno**

*Programa de Doctorado en Física y Matemáticas (FisyMat)*

Departamento de Física Atómica, Molecular y Nuclear  
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Granada, 9 de Abril de 2018

Fdo.: Jesús Sánchez-Dehesa Moreno-Cid.

Memoria presentada por David Puertas Centeno para optar al Grado de Doctor en Física por la Universidad de Granada.

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Al insondable misterio,  
del que emana el calor  
de la curiosidad

A la memoria de mi padre

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*Un entendimiento todo lógica es como un cuchillo hoja solo, que hiere la mano de su dueño.* **Rabindranath Tagore** (1861-1941) (NP 1913)

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# Summary

Multidimensional quantum systems consisting of many particles are a major challenge in Quantum Physics, since their behavior can be determined only with immense computational power. Physicists are trying to discover elegant notions and techniques to simplify the problem. The internal complexity of quantum systems, the uncertainty of their constituents beyond the Heisenberg one (i.e., beyond the standard deviation of the associated probability densities) and the dimensionality of their associated configuration spaces are the *leit motiv* of this Thesis.

The quantum many-particle systems are not merely complicated in the way that machines are complicated but they are intrinsically complex in ways that are fundamentally different from any product of design. The fundamental issue is to find quantifiers which are able to capture the intuitive idea that complexity lies between perfect order and perfect disorder [1, 2]. The formalization of this intuition is a non-trivial task. Most probably it cannot be formalized by a single complexity quantifier because of the so many facets of the term *complexity*. Based on Information Theory [3, 4] and Density Functional Theory [5, 6], various computable and operationally meaningful density-dependent measures have been proposed for the internal complexity of the many-electron systems: the entropy and complexity measures of the electron probability density of the system. The former ones (Fisher information, Shannon entropy) capture a single macroscopic facet of the internal disorder of the system. The latter ones capture two or more macroscopic facets of the quantum probability density which characterize the system, being the most relevant ones up until now the complexity measures of Cramer-Rao, Fisher-Shannon and LMC (Lopez-Ruiz-Mancini-Calvet) type, which are composed by two entropic factors [7].

Quantum uncertainties are not errors. Werner Heisenberg (NP 1932) in a seminal article [8] used the term *mean error* for the uncertainties in the position and momentum spaces, a terminology that evokes error theory and standard deviations. Even so, Heisenberg hailed the Kennard inequality [9],  $\Delta x \Delta p \geq 1/2$  (in natural units with  $\hbar = 1$ ), as the precise mathematical expression of the uncertainty principle [10] for one-dimensional quantum systems and apart from a few dissident voices, the physics community has followed him almost until recently. But considering the Kennard inequality as an adequate expression of the uncertainty principle is just another remnant of the old days

of quantum theory. Nowadays we have entropy-like functionals of the position and momentum probability densities, such as e.g. the Rényi and Shannon entropies, which are much more adequate uncertainty measures to mathematically formalize the Heisenberg uncertainty principle of Quantum Physics.

Space dimensionality  $D$  is a fundamental variable in the analysis of the structure and dynamics of quantum systems and phenomena. Basically this is because the wave functions of the quantum wave equations (Schrödinger, Dirac, . . .), and consequently all the chemical and physical properties of these systems crucially depend on the dimensionality [11]. In addition,  $D$  is the basic variable of a very useful strategy, the  $D$ -dimensional scaling method, which Dudley Herschbach (NP 1986) et al [12–14] have developed to study the atomic and molecular systems. This method requires to solve a finite many-electron problem in the ( $D \rightarrow \infty$ )-limit and then, perturbation theory in  $1/D$  is used to have an approximate result for the standard dimension ( $D = 3$ ), obtaining at times a quantitative accuracy comparable to the self-consistent Hartree–Fock calculations. Furthermore, it has been recently shown that space dimensionality is a physico-technological resource in a number of scientific and technological fields ranging from fluids [15, 16] to ion Coulomb crystals (i.e., ordered structures of atomic and molecular ions stored in ion traps at temperatures close to the absolute zero point) [17], quantum criticality [18, 19], quantum information science and quantum information technologies [20–27]. Nowadays, there is an increasing interest on the dimensional dependence of the entropic properties for the stationary states of the multidimensional quantum systems [1, 28–37] in order to contribute to the emergent informational representation of the quantum systems which extends and complements the standard energetic representation; to this respect, let us keep in mind that the entropic properties do not depend on the energy eigenvalues but on the eigenfunctions of the states.

**The goal of the Thesis** is twofold: the determination of the entropic uncertainty of the Coulomb and harmonic systems, and the quantification of complexity attributed to many-particle systems. The latter task is closely connected with evolution from order to disorder which is among the most important scientific challenges in the theory of complex systems [1, 2, 38–40]; that is, to quantify how simple or how complex are the multidimensional many-particle systems in terms of the information-theoretic measures of their one-particle probability density which, according to the Density Functional Theory, characterize their physical and chemical properties. In this dissertation we have first provided various novel multiparametric complexity measures, which extend and generalize the previous intrinsic complexities encountered in the literature. Then, we have analytically calculated and numerically discussed these complexity quantities and the entropic uncertainty measures of various multidimensional quantum phenomena and systems, such as the black body radiation in standard and non-standard universes and the multidimensional hydrogenic and harmonic systems, which are the reference systems in  $D$ -dimensional Coulomb and harmonic physics, respectively. Emphasis has been done

on the analytical side for the extreme stationary states of high-energy (Rydberg) and high-dimensional (pseudoclassical) types, whose numerical computation is a practically impossible task.

**The methodology of the Thesis** includes a diversity of methods extracted from Information Theory [3, 4, 30, 41, 42], Probability Theory [43], and algebraic and asymptotic techniques from Approximation Theory and the theory of orthogonal polynomials [44–55], hyperspherical harmonics [37, 56–58] and other special functions of Applied Mathematics and Mathematical Physics [46, 59].

**The structure of the Thesis**, presented in the modality of a collection of articles, is composed by two parts and seven chapters which are self-contained to a great extent. Part I, which contains an introduction and chapters 1–3, is devoted to the entropic uncertainty measures of the Coulomb and harmonic systems. Part II, which gathers an introduction and chapters 4–7, is devoted to the multiparametric complexity measures and their application to the generalized Planck distribution and hydrogenic and harmonic systems. Finally, some conclusions and open problems are given.

Chapter 1 has a methodological character. It contains (i) the basic dispersion and entropic notions of the multidimensional continuous probability distributions which we have used throughout the dissertation (see section 1.1), (ii) various mathematical theorems and propositions which give the degree and parameter asymptotics of various entropic functionals of the orthogonal hypergeometric polynomials which control the wave functions of the Coulomb and harmonic systems analyzed in this work (see section 1.2), and (iii) the scarcely known linearization methods of Srivastava type for the powers of these polynomials (see section 1.3) which will be used later on for the determination of the entropic uncertainty measures of Rényi type.

Chapter 2 is devoted to the analytical determination and discussion of the Rényi and Shannon entropies for the discrete stationary states of the multidimensional hydrogenic systems, with emphasis in the two following groups of extreme states: the highly-excited (Rydberg) and the high-dimensional (pseudoclassical). In Chapter 3 a similar work is done for the multidimensional harmonic systems.

Chapter 4 has a descriptive character. It contains a brief summary of the main two-factor complexity measures of the multidimensional continuous probability distributions used in the literature which have been applied in electronic structure and their generalizations [1, 7, 30, 60] as well as their inequality-type properties.

In Chapter 5 we introduce three biparametric measures of complexity for general continuous probability distributions and discuss their fundamental properties. Later on, we apply them to the multidimensional Planck distribution which characterizes the spectral frequency of the blackbody radiation at standard and non-standard universes.

In Chapter 6 we present the notion and the properties of a novel type of escort distributions for univariate probability distributions, the differential-escort distributions, which have a number of advantages with respect to the standard escort ones. Then, we illustrate its utility to prove the monotonicity property of the LMC-Rényi complexity measure and we study its behaviour of general distributions in the two extreme cases of minimal and very high complexity.

In Chapter 7 we introduce a triparametric Fisher-Rényi complexity for a univariate probability density  $\rho$  which is based on the biparametric extensions of the Fisher information and the Rényi entropies of  $\rho$ . This novel measure quantifies the combined balance of the spreading and the gradient contents of  $\rho$ , and has the three main properties of a statistical complexity: the invariance under translation and scaling transformations, and a universal bounding from below. For this purpose we use the Gagliardo-Nirenberg inequality, and a generalization of the Stam inequality is required, as well as the differential escort notion, which has been the keystone to obtain the sharp inequality, the expression of the minimizers and the exact value of the optimal bound.

**The main results of the Thesis** are given in chapters 2 and 3 of Part I, as well as in chapters 5, 6 and 7 of Part II. They correspond to the contents of two preprints and eight articles published (as indicated in the paragraph *Author's Publications*) in the following reviews: Journal of Physics A: Mathematical and Theoretical, Entropy (2), International Journal of Quantum Chemistry, Journal of Mathematical Physics, Journal of Statistical Mechanics: Theory and Experiment, Physica A: Statistical Mechanics and its Applications, European Physical Journal-Special Topics.

One more publication of the author, related to but not included in this Thesis, has appeared (as indicated in the paragraph *Author's Publications*) in the Journal of Statistical Mechanics: Theory and Experiment.

# Resumen

El estudio de los sistemas cuánticos multidimensionales de muchas partículas constituyen un reto de primer orden en Física Cuántica, debido fundamentalmente a que su comportamiento solo puede determinarse con una capacidad computacional inmensa. Actualmente los físicos tratan de descubrir ideas y técnicas elegantes para simplificar el problema. La *complejidad* interna de los sistemas cuánticos, la *incertidumbre* de sus constituyentes más allá de la formulación de Heisenberg (i.e., más allá de la desviación típica asociada a las densidades de probabilidad monoparticulares de posición y momento) y la *dimensionalidad* de los correspondientes espacios de configuración son el *leit motiv* de esta Tesis.

Los sistemas cuánticos de muchas partículas no son meramente complicados en el sentido en el que lo es una máquina, sino que son intrínsecamente complejos en el sentido de que son fundamentalmente diferentes a cualquier producto de diseño. La cuestión fundamental es encontrar cuantificadores que sean capaces de capturar la idea intuitiva de que la complejidad se encuentra comprendida entre el orden perfecto y el desorden total [1, 2]. La formalización de esta intuición es una tarea no-trivial. Lo más probable es que no pueda llevarse a cabo matemáticamente mediante un único cuantificador debido a las muchas facetas que tiene el término *complejidad*. En base a la Teoría de la Información [3, 4] y la Teoría Funcional de la Densidad [5, 6], se han propuesto varias medidas dependientes de la densidad, computables y operacionalmente significativas, para la complejidad intrínseca de los sistemas electrónicos: las medidas de entropía y complejidad de la densidad de probabilidad monoparticular del sistema. Las primeras (información de Fisher, entropía de Shannon) capturan una sola faceta macroscópica del desorden interno del sistema. Las últimas capturan dos o más facetas macroscópicas de la densidad de probabilidad cuántica que caracteriza al sistema, siendo las más relevantes hasta ahora las medidas de complejidad de tipo Cramer-Rao, Fisher-Shannon y LMC (López-Ruiz-Mancini-Calvet), que están compuestas por dos factores entrópicos [1, 7, 61].

La *incertidumbre cuántica* no es propiamente un error. Werner Heisenberg (NP 1932) en un artículo seminal [8] usó el término *error medio* para las incertidumbres en los espacios de posiciones y momentos, una terminología que evoca la teoría de errores y la desviación estándar. No obstante, Heisenberg eligió la desigualdad de Kennard [9],  $\Delta x \Delta p \geq 1/2$

(en unidades naturales con  $\hbar = 1$ ), como la expresión matemática precisa del principio de incertidumbre [10] para sistemas cuánticos monodimensionales y, salvo unas pocas voces disidentes, la comunidad física lo ha aceptado así hasta muy recientemente. Pero considerar la desigualdad de Kennard como una expresión adecuada del principio de incertidumbre es sólo otro remanente de los viejos tiempos de la teoría cuántica. Hoy en día tenemos funcionales entrópicos de las densidades de probabilidad de posiciones y momentos, tales como e.g. las entropías de Fisher, Rényi y Shannon, las cuales son medidas de incertidumbre mucho más adecuadas para formalizar matemáticamente el principio de incertidumbre de Heisenberg de la Física Cuántica.

La *dimensionalidad espacial*  $D$  es una variable fundamental en el análisis de la estructura y la dinámica de los sistemas y fenómenos cuánticos. Básicamente esto se debe a que las funciones de onda (o sea, las soluciones físicas de las ecuaciones de onda cuánticas de tipo Schrödinger, Dirac,...), y consecuentemente todas las propiedades físico-químicas de estos sistemas dependen crucialmente de la dimensionalidad [11]. Además,  $D$  es la variable básica de una estrategia muy útil, el método de escalamiento  $D$ -dimensional, que Dudley Herschbach (NP 1986) et al. [12–14] han desarrollado para estudiar los sistemas atómicos y moleculares. Este método requiere resolver un problema finito de muchos electrones en el límite ( $D \rightarrow \infty$ ) y después usar la teoría de perturbaciones en  $1/D$  para tener un resultado aproximado en la dimensión estándar ( $D = 3$ ); los resultados obtenidos presentan, en ocasiones, una exactitud cuantitativa comparable a los cálculos auto-consistentes de Hartree-Fock. Estas ideas están siendo utilizadas para estudiar numerosos sistemas y fenómenos físicos desde los fluidos reales [15, 16] y los cristales de iones coulombianos (i.e., estructuras ordenadas de iones atómicos y moleculares confinados en trampas iónicas a temperaturas cercanas al cero absoluto) [17] hasta la criticalidad cuántica [18, 19]. Además, se ha probado recientemente que la dimensionalidad espacial es un recurso físico-tecnológico en la ciencia y las tecnologías de la información cuántica [20–27]. Actualmente existe un creciente interés en la dependencia con la dimensionalidad de las propiedades entrópicas de los estados estacionarios de los sistemas cuánticos multidimensionales [1, 28–37] con el fin de contribuir a la emergente representación informacional de los sistemas cuánticos que extiende y complementa la representación energética estándar. A este respecto, ha de tenerse presente que las propiedades entrópicas no dependen de los autovalores de la energía sino de las autofunciones de los estados del sistema.

**El objetivo de esta Tesis** es doble: el análisis de la incertidumbre entrópica en los sistemas Coulombianos y armónicos, y la cuantificación de la complejidad de los sistemas de muchas partículas. Esta última tarea está estrechamente relacionada con la evolución del orden al desorden que es un desafío científico de primer nivel en la teoría de los sistemas complejos [1, 2, 38–40]. En esta disertación, primero proponemos nuevas medidas de complejidad multiparamétrica que extienden y generalizan las medidas de complejidad conocidas. Después calculamos analíticamente y discutimos numéricamente

estos cuantificadores de la complejidad y las medidas de incertidumbre entrópica en varios fenómenos y sistemas cuánticos multidimensionales, tales como la radiación de cuerpo negro en universos de dimensionalidad estándar y no-estándar y los sistemas hidrogenoideos y armónicos multidimensionales, que son los sistemas de referencia en la física D-dimensional coulombiana y armónica, respectivamente. Se hace énfasis en la determinación analítica de los cuantificadores teórico-informacionales de los estados estacionarios extremos de alta energía (Rydberg) y de alta dimensionalidad (pseudoclásicos), cuyo cálculo numérico es una tarea computacional prácticamente imposible.

**La metodología de la Tesis** incluye una gran diversidad de métodos procedentes de la Teoría de la Información Clásica y Cuántica [3, 4, 30, 41, 42] y de la Teoría de la Probabilidad [43], así como de técnicas algebraicas y asintóticas de la Teoría de Aproximación y de la teoría de los polinomios ortogonales [44–55], los armónicos hipersféricos [37, 56–58] y otras funciones especiales de la Matemática Aplicada y la Física Matemática [46, 59].

**La estructura de la Tesis**, que se presenta en la modalidad de agrupamiento de publicaciones, se compone de dos partes y siete capítulos que son autocontenidos en gran medida. La Parte I, que contiene los capítulos 1, 2 y 3, está dedicada a las medidas de incertidumbre entrópica de los sistemas armónicos y coulombianos. La Parte II, que abarca los capítulos 4, 5, 6, y 7, está dedicada a las medidas de complejidad multiparamétricas y su aplicación a la distribución de Planck generalizada y a los sistemas armónicos e hidrogenoideos. Finalmente, se dan algunas conclusiones y se señalan algunos problemas abiertos de forma no-exhaustiva.

El capítulo 1 tiene carácter metodológico. En él se describen (i) las nociones básicas de dispersión y entropía de distribuciones de probabilidad continuas multidimensionales que se usan en esta disertación (ver sección 1.1), (ii) varios teoremas y proposiciones matemáticas que describen la asintótica en el grado y en el parámetro de distintos funcionales entrópicos de los polinomios hipergeométricos ortogonales que controlan las funciones de onda de los sistemas coulombianos y armónicos analizados en este trabajo (ver sección 1.2), y (iii) los métodos de linealización de tipo Srivastava para las potencias de estos polinomios (ver sección 1.3) que serán después usados para la determinación de las medidas de incertidumbre entrópicas de tipo Rényi.

El capítulo 2 está dedicado a la determinación analítica y discusión de las entropías de Rényi y Shannon para los estados estacionarios discretos de los sistemas hidrogenoideos multidimensionales, haciendo hincapié en dos tipos de estados extremos: los estados altamente excitados (Rydberg) y los estados de gran dimensionalidad (pseudoclásicos). En el capítulo 3 se lleva a cabo un trabajo similar para los sistemas armónicos multidimensionales.

El capítulo 4 tiene un carácter descriptivo. En él se hace un breve resumen de las principales medidas de complejidad de densidades de probabilidad continuas multidimensionales de dos factores usadas en la literatura, las cuales han sido aplicadas en estructura electrónica para interpretar un gran número de fenómenos mecano-cuánticos de los sistemas atómicos y moleculares [1]. Se describen también las generalizaciones de estas medidas, así como sus propiedades de tipo desigualdad.

En el capítulo 5 introducimos tres medidas de complejidad biparamétricas para densidades de probabilidad generales y discutimos sus propiedades fundamentales. Después las aplicamos a la distribución de Planck generalizada que caracteriza el espectro de frecuencias de la radiación del cuerpo negro en universos de dimensionalidad estándar y no estándar.

En el capítulo 6 presentamos la noción y las propiedades de un nuevo tipo de distribuciones escort para densidades de probabilidad univaluadas, las distribuciones escort-diferenciales, que presentan ciertas ventajas con respecto a las escort estándar. Después mostramos su utilidad para probar la propiedad de monotonicidad de la medida de complejidad de LMC-Rényi y analizamos su comportamiento para distribuciones generales en los dos casos extremos de mínima y muy alta complejidad.

En el capítulo 7 introducimos la medida de complejidad de Fisher-Rényi triparamétrica para una densidad de probabilidad univaluada  $\rho$ . Esta nueva medida cuantifica el balance combinado del esparcimiento y el contenido en gradiente de  $\rho$ , y tiene las tres propiedades principales de una medida de complejidad estadística: la invarianza bajo transformaciones de escala y traslación y una cota mínima universal. Para ello ha sido necesario la utilización de la desigualdad de Gagliardo-Nirenberg con el fin de extraer una generalización de la desigualdad de Stam, así como la noción de transformación escort-diferencial, que ha sido la clave fundamental para obtener la expresión de las densidades minimizantes y el valor exacto de la cota óptima.

**Los resultados principales de la Tesis** se describen en los capítulos 2 y 3 de la Parte I, así como en los capítulos 5, 6 y 7 de la Parte II. Tales resultados han dado lugar, tal como se detalla en el apartado *Author's Publications*, a dos preprints y ocho artículos publicados en las revistas: Journal of Physics A: Mathematical and Theoretical, Entropy (2), International Journal of Quantum Chemistry, Journal of Mathematical Physics, Journal of Statistical Mechanics: Theory and Experiment, Physica A: Statistical Mechanics and its Applications, European Physical Journal-Special Topics.

Otra publicación del autor, relacionada con los tópicos de esta Tesis pero no incluida en ella, ha aparecido publicada en la revista Journal of Statistical Mechanics: Theory and Experiment, tal como se menciona también en el apartado *Author's Publications*.



# Author's publications

Since the Thesis is presented in the modality of a publications' collection, we list below the publications upon which this Thesis is based. Note that brackets at the end of each reference indicate the Chapters and/or Sections where they have been explicitly included. The reference number of the publications is also pointed out.

- Toranzo, I. V., **Puertas-Centeno, D.**, & Dehesa, J. S.  
*Entropic properties of  $D$ -dimensional Rydberg systems.*  
Physica A: Statistical Mechanics and its Applications 462, 1197-1206 (2016).  
(Sec. 2.1) [31]
- **Puertas-Centeno, D.**, Temme, N. M., Toranzo, I. V., & Dehesa, J. S.  
*Entropic uncertainty measures for large dimensional hydrogenic systems.*  
Journal of Mathematical Physics 58(10), 103302 (2017).  
(Sec. 2.2) [63]
- Dehesa, J. S., Toranzo, I. V., & **Puertas-Centeno, D.**  
*Entropic measures of Rydberg-like harmonic states.*  
International Journal of Quantum Chemistry 117(1), 48-56 (2017).  
(Sec. 3.1) [64]
- **Puertas-Centeno, D.**, Toranzo, I. V., & Dehesa, J. S.  
*Heisenberg and entropic uncertainty measures for large-dimensional harmonic systems.*  
Entropy 19(4), 164 (2017).  
(Sec. 3.2) [65]
- **Puertas-Centeno, D.**, Toranzo, I.V. and Dehesa, J.S.  
*Exact Rényi entropies of  $D$ -dimensional harmonic systems.*  
European Physical Journal-Special Topics (2018). Accepted.  
(Sec. 3.3) [66]
- **Puertas-Centeno, D.**, Toranzo, I. V., & Dehesa, J. S.  
*The biparametric Fisher–Rényi complexity measure and its application to the multidimensional blackbody radiation*

Journal of Statistical Mechanics: Theory and Experiment 2017(4) 043408 (2017).  
(Sec. 5.1) [67]

- **Puertas-Centeno, D.**, Toranzo, I. V., & Dehesa, J. S.  
*Biparametric complexities and generalized Planck radiation law.*  
Journal of Physics A: Mathematical and Theoretical 50(50), 505001 (2017).  
(Sec. 5.2) [68]

- Zozor, S., **Puertas-Centeno, D.**, & Dehesa, J. S.  
*On generalized Stam inequalities and Fisher–Rényi complexity measures.*  
Entropy 19(9), 493 (2017).  
(Chapter 7) [69]

\* \* \* \*

The following two preprints are also included in the Thesis.

- **Puertas-Centeno D.**, Toranzo I. V. and Dehesa J. S.  
*Analytical determination of position and momentum Rényi entropies for multidimensional hydrogenic systems.*  
Preprint UGR (2018). Submitted.  
(Sec. 2.3) [70]

- **Puertas-Centeno D.**  
*Differential escort distributions and LMC-Rényi complexity monotones.*  
Preprint UGR (2018). To be submitted.  
(Chapter 6) [71]

\* \* \* \*

Another related publication not included in this Thesis is the following:

- Sobrino-Coll, N., **Puertas-Centeno, D.**, Toranzo, I. V., & Dehesa, J. S.  
*Complexity measures and uncertainty relations of the high-dimensional harmonic and hydrogenic systems.*  
Journal of Statistical Mechanics: Theory and Experiment 2017(8), 083102 (2017).  
[34]

## Part I

# Entropic uncertainty of multidimensional quantum systems

# Introduction

Uncertainty is the word which better defines our time but it is very difficult to introduce it into our mathematical models. Perhaps this is because it is a primary concept of the same category as e.g. energy, information and complexity. So, it has many different facets which are characterized by a variety of physico-mathematical quantities, the uncertainty measures. Since the early times of quantum mechanics [8, 10], the standard deviation has been considered as an obvious measure of uncertainty in quantum mechanics. Heisenberg used it to express the first precise mathematical formalization of the position-momentum Quantum Uncertainty Principle in the form of the so-called Kennard inequality [9].

Actually, however, the standard deviation is neither a natural nor a generally adequate measure of quantum uncertainty so that the Kennard inequality, though mathematically correct, is not always an adequate expression of the uncertainty principle. The reason for this inadequacy is because the standard deviation gives a large weight to the tails of the probability distribution. This strong tail dependence of the standard deviation is not relevant when the tails fall off exponentially, as for a Gaussian or quasi-Gaussian distribution, but the probabilities associated to an arbitrary quantum-mechanical wave function are not generally of this type.

The advent of Information Theory [3, 4] leads to the introduction of various information entropies (e.g., Fisher information and Shannon, Rényi and Tsallis entropies) as more appropriate measures of uncertainty. The amount of information which one obtains by observing the result of an experiment depending on chance, can be taken numerically equal to the amount of uncertainty concerning the outcome of the experiment before carrying it out. Opposite to the standard deviation, these entropic uncertainty measures do not depend on a specific point of the support of the probability distribution. It is amazing the scarce knowledge about these quantities for multidimensional quantum systems taken into account their relevance in so many fields like e.g. atomic and molecular physics [12, 14, 30], quantum information science and quantum technologies [25, 26] and string theory [72]. Indeed, of all the grand attempts to establish an ultimate theory of particles and forces of nature, none has been as popular, ambitious and controversial as the theory of superstrings living in a space-time of many dimensions; perhaps five or eleven according to Kaluza-Klein and Hawking, respectively. There are authors who

hope that the eleven-dimensional supergravity theory is a strong candidate for a theory of everything in the sense that it might be a complete, consistent and unified theory which would describe all possible interactions.

This Part of the Thesis is devoted to the description of the main entropic uncertainty measures of multidimensional quantum physics and their exact determination for the main prototypes of the multidimensional Coulomb and harmonic systems; namely, the multidimensional hydrogenic and harmonic (oscillator-like) systems, respectively.

Three chapters compose Part I. In Chapter 1, we first give in Section 1.1 the main entropic uncertainty measures of the multidimensional probability distributions and the associated mathematical formalizations of the uncertainty principle, the so-called uncertainty relations, for general and central (i.e., spherically-symmetric) quantum-mechanical potentials. In Section 1.2 we briefly describe some known asymptotical methods for the hypergeometric orthogonal polynomials, which are later used to calculate the entropic uncertainty measures of some extreme states: the highly-excited states and the high-dimensional states of the quantum systems of hydrogenic and harmonic types. And in Section 1.3 we gather some linearization methods for powers of hypergeometric orthogonal polynomials, which are later used to determine the entropic uncertainty measures of Rényi type for Coulomb and harmonic systems.

In Chapters 2 and Chapter 3 we use the previous entropic notions and mathematical methodology to determine the uncertainty measures of Rényi and Shannon types for the Rydberg and pseudoclassical states and for the general discrete stationary states of the hydrogenic and harmonic systems, respectively.

# Chapter 1

## Entropy measures and orthogonal polynomials

In this chapter we give the dispersion and entropic notions together with the main mathematical tools used in Part I to determine the entropic uncertainty measures for the stationary states of the multidimensional Coulomb and harmonic systems, with emphasis in the Rydberg (i.e., high energy) and pseudo-classical (i.e., high dimensional) states. The chapter is composed of three sections: In Sec. 1.1, the very notions of Heisenberg-like measure, Shannon entropy, Fisher information and the Rényi and Tsallis entropies will be presented together with some generalizations, and the associated uncertainty properties will be discussed. In Sec. 1.2, the asymptotical methods for the orthogonal polynomials which control the quantum-mechanical wave functions of the hydrogenic and harmonic systems, namely the Laguerre and Gegenbauer polynomials, will be presented. Finally, in Sec. 1.3, the linearization methods for the integer powers of the orthogonal polynomials used in this work will be described.

### 1.1 Information entropies and their uncertainty properties

The physical properties of a single-particle  $d$ -dimensional quantum system are controlled by means of the spatial delocalization of the single-particle density  $\rho(\vec{r}) = |\Psi(\vec{r})|^2$ ,  $\vec{r} = (x_1, \dots, x_d) \in \Delta \subseteq \mathbb{R}_d$ , being  $\Psi(\vec{r})$  the physical solution of the Schrödinger equation of the system in position space. In the following  $\gamma(\vec{p})$ ,  $\vec{p} = (p_1, \dots, p_d)$ , denotes the probability density in momentum space so that  $\gamma(\vec{p}) = |\tilde{\Psi}(\vec{p})|^2$  where  $\tilde{\Psi}(\vec{p})$  denotes the  $d$ -dimensional Fourier transform of  $\Psi(\vec{r})$ .

Here we will gather the notions and some properties of the Shannon, Rényi and Tsallis entropies and Fisher information of  $d$ -dimensional quantum systems which describe the uncertainty of their single-particle density in a more appropriate manner than the

Heisenberg-like quantities given by the radial expectation values

$$\langle r^2 \rangle = \int_{\mathbb{R}_d} |\vec{r}|^2 \rho(\vec{r}) d\vec{r}, \quad \langle p^2 \rangle = \int_{\mathbb{R}_d} |\vec{p}|^2 \gamma(\vec{p}) d\vec{p} \quad (1.1)$$

These Heisenberg-like uncertainty measures in position and momentum spaces have allowed for the first mathematical formalizations [35, 73] of the position-momentum uncertainty principle of Quantum Physics as

$$\langle r^2 \rangle \langle p^2 \rangle \geq \frac{d^2}{4} \quad (1.2)$$

which are the straightforward generalization of the primitive Kennard inequality mentioned above, with the assumption  $\langle \vec{r} \rangle = \langle \vec{p} \rangle = 0$ . This uncertainty relation has been generalized by means of the radial expectation values of arbitrary order  $\langle r^\alpha \rangle$  and  $\langle p^\beta \rangle$  obtaining [35, 74–76] the inequality

$$\langle r^\alpha \rangle^{\frac{2}{a}} \langle p^\beta \rangle^{\frac{2}{b}} \geq C(a, b) = \max_{\alpha \in A} B(\alpha) M(a, \alpha) M(b, \alpha^*) \quad (1.3)$$

where  $B(\alpha)$  is

$$B(\alpha) = \frac{\alpha^{\frac{1}{\alpha-1}} \alpha^*{}^{\frac{1}{\alpha^*-1}}}{4e^2} \quad \text{for } \alpha \neq 1 \quad \text{y} \quad B(1) = \frac{1}{4}, \quad (1.4)$$

$\alpha^* = \alpha/(2\alpha - 1)$ ,

$$A = \left( \max \left( \frac{1}{2}, \frac{d}{d+a} \right); 1 \right], \quad (1.5)$$

and the function  $M$  has the form

$$M(l, \lambda) = \begin{cases} 2\pi e \left( \frac{l}{\Omega B \left( \frac{d}{l}, 1 - \frac{\lambda}{\lambda-1} - \frac{d}{l} \right)} \right)^{\frac{2}{d}} \left( \frac{-d(\lambda-1)}{d(\lambda-1) + l\lambda} \right)^{\frac{2}{l}} \left( \frac{l\lambda}{d(\lambda-1) + l\lambda} \right)^{\frac{2}{d(\lambda-1)}}, & 1 - \frac{l}{l+d} < \lambda < 1 \\ 2\pi e \left( \frac{l}{\Omega \Gamma \left( \frac{d}{l} \right)} \right)^{\frac{2}{d}} \left( \frac{d}{le} \right)^{\frac{2}{l}}, & \lambda = 1 \\ 2\pi e \left( \frac{l}{\Omega B \left( \frac{d}{l}, \frac{\lambda}{\lambda-1} \right)} \right)^{\frac{2}{d}} \left( \frac{d(\lambda-1)}{d(\lambda-1) + l\lambda} \right)^{\frac{2}{\lambda}} \left( \frac{l\lambda}{d(\lambda-1) + l\lambda} \right)^{\frac{2}{d(\lambda-1)}}, & \lambda > 1 \end{cases} \quad (1.6)$$

with  $\Omega = \frac{2\pi^{d/2}}{\Gamma(d/2)}$  and the Beta function  $B(x, y)$  [59]. A detailed study of the accuracy of this relation (1.3) is carried out in [35] for various prototypical  $d$ -dimensional systems. Note that in the case  $a = b = 2$  boils down to the previous expression (1.2)

The Shannon entropy of the  $d$ -dimensional quantum probability density  $\rho(\vec{r})$  is known [77, 78] to be given by the following logarithmic functional of the density

$$S[\rho] = - \int_{\mathbb{R}^d} \rho(\vec{r}) \log \rho(\vec{r}) d\vec{r}. \quad (1.7)$$

This quantity is not only relevant in information theory and quantum physics but also in numerous areas of mathematics, statistics, science and technology (see e.g. [79, 80]). The Shannon entropy becomes the well-known thermodynamical entropy in the case of a thermal ensemble [81]. It is worth noting that, unlike the more familiar entropy  $-\sum_i p_i \ln p_i$  (also due to Shannon) of a probability on a discrete sample space,  $S[\rho]$  can have any values in  $[-\infty, \infty]$ . Any sharp peaks in  $\rho(\vec{r})$  will tend to make  $S[\rho]$  negative, whereas positive values for  $S[\rho]$  are provoked by a slowly decaying tail; hence the Shannon entropy  $S[\rho]$  is a measure of how localized [78] the density  $\rho(\vec{r})$  is. Moreover, this measure of uncertainty fulfills a number of important properties [77, 81], highlighting the following position-momentum uncertainty relation [78, 82, 83]

$$S[\rho] + S[\gamma] \geq d(1 + \ln \pi), \quad (1.8)$$

where  $S[\gamma]$  denotes the momentum Shannon entropy of the system. This Shannon-entropy-based uncertainty relation is a more appropriate mathematical formalization of the position-momentum uncertainty principle, which expresses that the total uncertainty in position and momentum is necessarily bigger than the value  $d(1 + \ln \pi)$  for any quantum state of the system. Moreover, assuming the quantum-mechanical potential  $V_D(r)$  to be central (i.e., spherically symmetric) Rudnicki et al [84] have improved the previous entropic uncertainty relation as

$$S[\rho] + S[\gamma] \geq B_{l,\{\mu\}} \quad (1.9)$$

where the lower bound is

$$\begin{aligned} B_{l,\{\mu\}} = & 2l + d + 2 \ln \left[ \frac{\Gamma(l + \frac{d}{2})}{2} \right] - (2l + d - 1) \psi \left( l + \frac{d}{2} \right) \\ & + (d - 1) \left[ \psi \left( \frac{2l + d}{4} \right) + \ln 2 \right] + 2 S(\mathcal{Y}_{l,\{\mu\}}), \end{aligned}$$

The symbol  $\psi(x)$  denotes the digamma function [59]), and the symbol  $\mathcal{Y}_{l,\{\mu\}}(\Omega_{d-1})$  denotes the hyperspherical harmonics [41, 85] characterized by the  $d - 1$  hyperangular quantum numbers  $(l \equiv \mu_1, \mu_2, \dots, \mu_{d-1} \equiv m) \equiv (l, \{\mu\})$ , which are integer numbers with values  $l = 0, 1, 2, \dots$ , and  $l \geq \mu_2 \geq \dots \geq \mu_{d-2} \geq |\mu_{d-1}| \geq 0$ . Notice that for  $d = 2$  we only have one quantum number  $l \in \mathbb{Z}$ . Moreover, the symbol  $S(\mathcal{Y}_{l,\{\mu\}})$  denotes [85] the Shannon-type entropic functional of the well-known hyperspherical harmonics  $S(\mathcal{Y}_{l,\{\mu\}})$  which are under control in the sense that they do not depend on the analytical form of the potential and so, they can be calculated both numerically and analytically [84]. The



bound (1.8) depends on the dimensionality  $d$  and on the angular hyperangular numbers  $\{\mu_i, i = 1, \dots, d-1\}$  of the quatum state of the system, but not on the hyperquantum principal number because the explicit analytical form of the potential is unknown.

The Rényi entropies  $R_q[\rho]$  [43, 86] and the Tsallis entropies  $T_q[\rho]$  [87], which are monoparametric extensions of the Shannon entropy, are defined by

$$R_q[\rho] = \frac{1}{1-q} \ln \left( \int_{\mathbb{R}^d} [\rho(\vec{r})]^q d\vec{r} \right); \quad q > 0, q \neq 1 \quad (1.10)$$

and

$$T_q[\rho] = \frac{1}{1-q} \left( 1 - \int_{\mathbb{R}^d} [\rho(\vec{r})]^q d\vec{r} \right); \quad q > 0, q \neq 1, \quad (1.11)$$

respectively. Note that in the limit  $q \rightarrow 1$ , both entropies reduce to the Shannon entropy  $S[\rho]$ . It is interesting to remark that these three quantities are global measures of spreading of the density  $\rho(\vec{r})$  because they are power (Rényi, Tsallis) and logarithmic (Shannon) functionals of  $\rho(\vec{r})$ . The Rényi entropies are additive while the Tsallis entropies are non-negative, extremal at equiprobability, concave for  $q > 0$  and pseudoadditive (i.e.  $T_q[\rho_1 \otimes \rho_2] = T_q[\rho_1] + T_q[\rho_2] + (1-q)T_q[\rho_1]T_q[\rho_2]$ ). Moreover, both Rényi and Tsallis entropies characterize separately the probability density under certain Hamburger-like conditions [88, 89]. Finally, most interesting is that they allow for the following mathematical formalizations of the quantum uncertainty principle found by Rajagopal [90]

$$\{1 + (1-p)T_p[\rho]\}^{\frac{-1}{2p}} \times \{1 + (1-q)T_q[\gamma]\}^{\frac{1}{2q}} \geq \left(\frac{q}{\pi}\right)^{\frac{d}{4q}} \left(\frac{p}{\pi}\right)^{\frac{-d}{4p}} \quad (1.12)$$

(with  $\frac{1}{q} + \frac{1}{p} = 2$ ) for Tsallis entropies, and by Bialynicki-Birula, Zozor and Vignat [91–94]

$$R_p[\rho] + R_q[\gamma] \geq d \log \left( \pi p^{\frac{1}{2(p-1)}} q^{\frac{1}{2(q-1)}} \right), \quad (1.13)$$

for the Rényi entropies, respectively. For completeness, let us point out that although the case out of the conjugation curve  $\frac{1}{p} + \frac{1}{q} > 2$  have been proved to be a non-trivial bound [93] the *sharp* bound in this case is not known yet. Recently, Dehesa et al [95] have heuristically obtained the Rényi-entropy-based uncertainty relation 1.13 can be improved as

$$R_p[\rho] + R_q[\gamma] \geq \frac{2p \ln A(2p)}{p-1} + \frac{2q \ln A(2q)}{q-1} + R_p(\mathcal{Y}) + R_q(\mathcal{Y})$$

for  $d$ -dimensional physical systems subject to a central quantum-mechanical potential, where the  $A$ -constant is given by

$$A(q) = \frac{2^{\frac{2-d}{2q}} q^{\frac{lq+d}{2q}}}{\Gamma\left(\frac{1}{2}(lq+d)\right)^{\frac{1}{q}}}$$

and the symbol  $R_p(\mathcal{Y})$  denote the Rényi-like integral functional of the hyperspherical harmonics  $\mathcal{Y}_{l,\{\mu\}}(\Omega_{d-1})$ , which is under control in the sense we have mentioned above. Let us comment that this lower bound improves the general lower bound, finding moreover that in the limit  $p, q \rightarrow 1$  the new bound for central potentials boils down to the Shannon-entropy-based lower bound (1.9) valid for central potentials, as one would expect.

The (translationally invariant) Fisher information of the  $d$ -dimensional probability density  $\rho(\vec{r})$  is defined [41] by the following gradient functional of the density

$$F[\rho] = \int_{\mathbb{R}^d} \rho(\vec{r}) \left| \vec{\nabla}_d \log \rho(\vec{r}) \right|^2 d\vec{r} = \int_{\mathbb{R}^d} \frac{\left| \vec{\nabla}_d \rho(\vec{r}) \right|^2}{\rho(\vec{r})} d\vec{r}, \quad (1.14)$$

where  $\vec{\nabla}_d$  denotes the  $d$ -dimensional gradient of the particle. The corresponding quantity for the momentum-space probability density  $\gamma(\vec{p})$  will be denoted by  $F[\gamma]$ . This concept was firstly introduced for one-dimensional random variables in statistical estimation [96] but nowadays it is playing an increasing role in numerous fields [97–104], including electronic structure; this is partially because of its formal resemblance with kinetic [97, 105–107] and Weiszäcker [6, 108] energies. The Fisher information, contrary to the Shannon entropy (and its generalizations of e.g. Rényi and Tsallis types), is a local measure of spreading of the density  $\rho(\vec{r})$  because it is a gradient functional of  $\rho(\vec{r})$ . The higher this quantity is, the more localized is the density, the smaller is the uncertainty and the higher is the accuracy in predicting the localization of the particle. It has, however, an intrinsic connection with various spreading measures (variance, Shannon's entropy) by means of a number of celebrated information-theoretic inequalities such as e.g. the de Bruijn inequality [3, 109], the Stam-like inequalities [110–112] and the Cramer-Rao inequality [3, 109, 113].

The notion of Fisher information has been shown to be very fertile to identify, characterize and interpret numerous phenomena and processes in atomic and molecular physics such as e.g., correlation properties in atoms, spectral avoided crossings of atoms in external fields [98], the periodicity and shell structure in the periodic table of chemical elements [111] and the transition state and other stationary points in chemical reactions [113]. Moreover, it has been used for the variational characterization of quantum equations of motion [97] as well as to rederive the classical thermodynamics without requiring the usual concept of Boltzmann's entropy [114]. Most important for our purposes is to highlight that the Fisher information allows us to obtain [115] another mathematical formalization of the position-momentum uncertainty principle in the form of the uncertainty relation

$$F[\rho] \times F[\gamma] \geq 4d^2, \quad (1.15)$$

where  $F[\gamma]$  denotes the Fisher information of the  $d$ -dimensional quantum system in

momentum space. Moreover, for quantum systems with a central potential the position-momentum Fisher uncertainty product is related [116] to the Heisenberg uncertainty product as

$$F[\rho] \times F[\gamma] \geq 16 \left[ 1 - \frac{(2l + d - 2)|m|}{2l(l + d - 2)} \right]^2 \langle r^2 \rangle \langle p^2 \rangle, \quad (1.16)$$

(where  $r^2 = x_1^2 + x_2^2 + \dots + x_D^2$  and  $p^2 = p_1^2 + p_2^2 + \dots + p_D^2$ ) which illustrates the uncertainty character of the Fisher-information product  $F[\rho] \times F[\gamma]$ . Moreover, by using (1.16) and the general Heisenberg-like inequality for  $d$ -dimensional quantum-mechanical potentials

$$\langle r^2 \rangle \langle p^2 \rangle \geq \left( l + \frac{d}{2} \right)^2 = \left( L + \frac{3}{2} \right)^2, \quad (1.17)$$

we obtain [117] the following Fisher-information-based uncertainty relation

$$F[\rho] \times F[\gamma] \geq 16 \left[ 1 - \frac{(2l + d - 2)|m|}{2l(l + d - 2)} \right]^2 \left( l + \frac{d}{2} \right)^2 \quad (1.18)$$

which extends and improves a similar relation previously obtained in three [118] and  $d$  [116] dimensions. Note that the equality is reached for the ground-state oscillator wavefunctions. Moreover, for  $S$  states (i.e. when  $l = 0$ ), this inequality boils down to Eq. (1.15). This illustrates the improvement of Eq. (1.18) with respect to Eq. (1.15) due to consideration of the spherical symmetry.

Finally, let us mention here for completeness that the Fisher notion has been extended to the biparametric case for one-dimensional probability densities by Lutwak et al [119], and more recently for multi-dimensional probability densities by Bercher [120] and Lutwak et al [121] as

$$F_{p,\lambda}[\rho] = \int_{\mathbb{R}_d} \rho(\vec{r}) \left( \rho(\vec{r})^{\lambda-2} |\vec{\nabla} \rho(\vec{r})| \right)^p d\vec{r}, \quad (1.19)$$

These quantities will not be analyzed in this Part but in Part II, where some properties will be taken into account and novel quantities of similar type will be proposed. It is interesting to remark that no uncertainty relations associated to this generalized Fisher information have been encountered yet. Let us comment that for pure convenience we use, at times, the quantity  $\phi_{p,\lambda}[\rho] = F_{p^*,\lambda}[\rho]^{\frac{1}{p^*\lambda}}$  where  $p^*$  is the conjugated number of  $p$  in the following sense  $\frac{1}{p} + \frac{1}{p^*} = 1$ .

## 1.2 Asymptotics for integral functionals of orthogonal polynomials

In this section we briefly review the asymptotical methods for orthogonal polynomials used in this work. First, in subsection 1.2.1, we give the Theorem of Aptekarev et al [122] which describes the asymptotics of the Rényi-type integral functionals of the Laguerre polynomials  $L_n^{(\alpha)}(x)$ ,  $\alpha > -1$ , (see e.g., [59]) in the limit of a very large degree

$n \gg 1$ . This theorem, which is an extension of a previous similar result for integral functionals of Hermite polynomials [50], allows to calculate the radial part of the physical Rényi entropies for the highly and very highly excited states of both multidimensional harmonic and hydrogenic systems [31, 64, 122]. Then, in subsection 1.2.2, we state the Theorems of Temme et al [123] which describe the asymptotics of of the Rényi-type and Shannon-type integral functionals of the Laguerre and Gegenbauer polynomials when the parameter is very large,  $\alpha \gg 1$ . These quantities control the physical Rényi and Shannon entropies for the pseudo-classical states (i.e., the highest dimensional states) of the multidimensional harmonic and hydrogenic systems [63, 65].

### 1.2.1 Degree asymptotics of Laguerre entropic functionals

The Rényi-like integral functional,  $N_n(D, p)$ , of the orthonormal Laguerre polynomials  $\hat{L}_n^{(\alpha)}(x)$  with respect to the weight function  $\omega_\alpha(x) = x^\alpha e^{-x}$ ,  $\alpha > -1$ , on the interval  $[0, \infty)$ , given by

$$N_n(D, p) = \int_0^\infty \left( [\hat{L}_n^{(\alpha)}(x)]^2 \omega_\alpha(x) \right)^p x^\beta dx, \quad p > 0, \quad (1.20)$$

essentially controls the behaviour of the physical Rényi entropies for all the stationary states of the  $D$ -dimensional harmonic systems in both position and momentum spaces [64] and of the  $D$ -dimensional hydrogenic systems in position space [122]. In the hydrogenic case one has  $\alpha = 2l + D - 2$ , with  $l = 0, 1, 2, \dots, n - 1$ , and  $\beta = (2 - D)p + D - 1$ , while in the oscillator-like (i.e., harmonic) case one has  $\alpha = l + \frac{1}{2}$ ,  $l = 0, 1, 2, \dots$ , and  $\beta = \frac{1}{2}(1 - p)$ . Note that the condition  $\beta + p\alpha > -1$ , required for the convergence of the integral, is satisfied for all physical parameters.

In this subsection we give the asymptotics of the integral functionals  $N_n(D, p)$  of Laguerre polynomials for the hydrogenic and harmonic sets of parameters  $(\alpha, l, \beta)$  just mentioned in the form of the two following theorems, recently found .

**Theorem 1.1.** [122] *The asymptotics ( $n \rightarrow \infty$ ) of the Rényi-type Laguerre hydrogenic functionals  $N_{n,l}^{(H)}(D, p)$  defined by Eq. (1.20) with the parameters  $\alpha = 2l + D - 2$ , with  $l = 0, 1, 2, \dots, n - 1$ , and  $\beta = (2 - D)p + D - 1$ , is given for all possible values of  $D$  and  $p > 0$  as follows:*

1. If  $\beta > 0$ , there are two subcases:

(a) If  $D > 2$ , and  $p \in \left(0, \frac{D-1}{D-2}\right)$  then

$$N_{n,l}^{(H)}(D, p) = C(\beta, p) (2(n - l - 1))^{1+\beta-p} (1 + \bar{o}(1)),$$

(b) If  $D = 2$  (so,  $\beta = 1$ ), then

$$N_{n,l}^{(H)}(D, p) = \begin{cases} C(1, p) (2(n-l-1))^{2-p} (1 + \bar{o}(1)), & p \in (0, 2) \\ \frac{\ln(n-l-1) + \underline{Q}(1)}{\pi^2}, & p = 2 \\ \frac{C_A(p)}{\pi^p} (4(n-l-1))^{\frac{2}{3}(2-p)} (1 + \bar{o}(1)) & p \in (2, 5) \\ \left( \frac{C_A(p)}{\pi^p 4^2} + C_B(\alpha, 1, p) \right) (n-l-1)^{-2}, & p = 5 \\ C_B(\alpha, 1, p) (n-l-1)^{-2}, & p \in (5, \infty). \end{cases}$$

2. If  $\beta = 0$  (so,  $D \neq 2$  and  $p = \frac{D-1}{D-2}$ ), then

$$N_{n,l}^{(H)}(D, p) = \begin{cases} C(0, p) (2(n-l-1))^{(1-p)} (1 + \bar{o}(1)), & p = \frac{D-1}{D-2} \\ \frac{\ln(n-l-1) + \underline{Q}(1)}{\pi^2(n-l-1)}, & p = 2, (D = 3). \end{cases}$$

3. If  $\beta < 0$  (so, either  $p < \frac{D-1}{D-2}$  and  $D < 2$  or  $p > \frac{D-1}{D-2}$  and  $D > 2$ ), then

$$N_{n,l}^{(H)}(D, p) = \begin{cases} C(\beta, p) (2(n-l-1))^{1+\beta-p} (1 + \bar{o}(1)), & p \in \left( \frac{D-1}{D-2}, \frac{2D}{2D-3} \right) \\ \frac{2\Gamma(p+1/2) (\ln n + \underline{Q}(1))}{\pi^{p+1/2} \Gamma(p+1) (4(n-l-1))^{1+\beta}}, & p = 2 + 2\beta = \frac{2D}{2D-3}, \\ C_B(\alpha, \beta, p) (n-l-1)^{-(1+\beta)} (1 + \bar{o}(1)), & p > 2 + 2\beta = \frac{2D}{2D-3} \end{cases}$$

where the constants  $C, C_B, C_A$  are given by

$$C(\beta, p) := \frac{2^{\beta+1}}{\pi^{p+1/2}} \frac{\Gamma(\beta+1-p/2) \Gamma(1-p/2) \Gamma(p+1/2)}{\Gamma(\beta+2-p) \Gamma(1+p)},$$

$$C_A(p) := \int_{-\infty}^{+\infty} \left[ \frac{2\pi}{\sqrt[3]{2}} \text{Ai}^2 \left( -\frac{t\sqrt[3]{2}}{2} \right) \right]^p dt,$$

and

$$C_B(\alpha, \beta, p) := 2 \int_0^{\infty} t^{2\beta+1} |J_{\alpha}(2t)|^{2p} dt,$$

respectively. The symbols  $\text{Ai}(t)$  and  $J_{\alpha}(z)$  denote the Airy and the Bessel functions (see [59, 124]) defined by

$$\text{Ai}(y) = \frac{\sqrt[3]{3}}{\pi} A(-3\sqrt{3}y), \quad A(t) = \frac{\pi}{3} \sqrt{\frac{t}{3}} \left[ J_{-1/3} \left( 2 \left( \frac{t}{3} \right)^{\frac{3}{2}} \right) + J_{1/3} \left( 2 \left( \frac{t}{3} \right)^{\frac{3}{2}} \right) \right].$$

and

$$J_{\alpha}(z) = \sum_{\nu=0}^{\infty} \frac{(-1)^{\nu}}{\nu! \Gamma(\nu + \alpha + 1)} \left( \frac{z}{2} \right)^{\alpha+2\nu}.$$

respectively.

A similar result can be obtained for the asymptotics ( $n \rightarrow \infty$ ) of the Laguerre oscillator-like (harmonic) functionals  $N_{n,l}^{(O)}(D,p)$  defined by Eq. (1.20) with the parameters  $\alpha = l + \frac{D}{2} - 1$  and  $\beta = (p-1)(1 - \frac{D}{2})$ . This  $D$ -dimensional oscillator-like asymptotical result can be expressed for three-dimensional systems as follows:

**Theorem 1.2.** [64, 122] *The asymptotics ( $n \rightarrow \infty$ ) of the Rényi-type Laguerre oscillator-like (i.e., harmonic) functionals  $N_{n,l}(D,p)$  defined by Eq. (1.20) with the parameters  $D = 3, \alpha = l + \frac{1}{2}, l = 0, 1, 2, \dots$ , and  $\beta = \frac{1}{2}(1 - p)$  is given by*

$$N_{n,l}^{(O)}(3,p) = \begin{cases} \lambda^{\frac{3}{2}(p-1)} C(\beta,p) (2n^3)^{\frac{1-p}{2}} (1 + \bar{o}(1)), & p \in (0, p^*) \\ \lambda^{3/4} \frac{8\sqrt{2}}{3\pi^{5/2}} n^{-3/4} (\ln n + \underline{O}(1)), & p = p^* \\ (2\lambda^{\frac{3}{2}})^{p-1} C_B(\alpha, \beta, p) n^{(p-3)/2} (1 + \bar{o}(1)), & p > p^* \end{cases}, \quad (1.21)$$

with  $p^* = \frac{3}{2}$ .

This theorem will be used to determine the Rényi entropies for the Rydberg states of both three-dimensional Coulomb (see Sec. 2.1) and harmonic systems (see Sec. 3.1).

### 1.2.2 Parameter asymptotics of Laguerre and Gegenbauer entropic functionals

In this subsection the asymptotics ( $\alpha \rightarrow \infty$ ) of some Rényi-like integral functionals of the orthogonal Laguerre polynomials  $\mathcal{L}_n^{(\alpha)}(x)$  and Gegenbauer polynomials  $\mathcal{C}_n^{(\alpha)}(x)$  is given by means of the two following theorems recently found by Temme et al [123]. They will be later used to determine the physical Rényi entropies for the pseudoclassical states (i.e., the highest dimensional states) of both  $D$ -dimensional hydrogenic (Sec. 2.2) and harmonic systems (Sec. 3.2).

**Theorem 1.3.** [123] *Let  $\alpha, \kappa$  be positive real numbers,  $0 < \lambda \neq 1, \sigma$  real and  $m$  a positive natural number. Then, the Rényi-type functional of the Laguerre polynomials  $\mathcal{L}_m^{(\alpha)}(x)$*

$$J_1(\sigma, \lambda, \kappa, m; \alpha) = \int_0^\infty x^{\alpha+\sigma-1} e^{-\lambda x} \left| \mathcal{L}_m^{(\alpha)}(x) \right|^\kappa dx \quad (1.22)$$

has the following ( $\alpha \rightarrow \infty$ )-asymptotic behavior

$$J_1(\sigma, \lambda, \kappa, m; \alpha) \sim \alpha^{\alpha+\sigma} e^{-\alpha} \lambda^{-\alpha-\sigma-\kappa m} |\lambda - 1|^{\kappa m} \sqrt{\frac{2\pi}{\alpha}} \frac{\alpha^{\kappa m}}{(m!)^\kappa} \sum_{j=0}^\infty \frac{D_j}{\alpha^j}, \quad (1.23)$$

with the first coefficients  $D_0 = 1$  and

$$D_1 = \frac{1}{12(\lambda-1)^2} \left( 1 - 12\kappa m \sigma \lambda + 6\sigma^2 \lambda^2 - 12\sigma^2 \lambda - 6\sigma \lambda^2 + 12\sigma \lambda + 6\kappa^2 m^2 + 12\kappa m \sigma - 12\kappa m^2 \lambda - 12\kappa m \lambda + 6\kappa m \lambda^2 + 6\kappa m^2 \lambda^2 + \lambda^2 + 6\sigma^2 - 2\lambda - 6\sigma + 6\kappa m^2 \right). \quad (1.24)$$

Moreover, in the particular case  $\lambda = 1$  and  $\kappa = 2$ , i.e. for the functional

$$J_1(\sigma, 1, 2, m; \alpha) = \int_0^\infty x^{\alpha+\sigma-1} e^{-x} \left| \mathcal{L}_m^{(\alpha)}(x) \right|^2 dx \quad (1.25)$$

we have the  $(\alpha \rightarrow \infty)$ -asymptotic behavior

$$I_5(m, \alpha) \sim \frac{\alpha^{\alpha+\sigma+m} e^{-\alpha}}{m!} \sqrt{\frac{2\pi}{\alpha}}. \quad (1.26)$$

See [123] for further details including the knowledge of the remaining coefficients and the proof of the theorem.

**Theorem 1.4.** [123] *Let  $a, b, c, d$ , and  $\kappa$  be positive real numbers,  $c < d$ , and  $m$  a positive natural number. Then, the Rényi-type functional of the Gegenbauer polynomials  $\mathcal{C}_m^{(\alpha)}(x)$  given by*

$$J_2(a, b, c, d, \kappa, m; \alpha) = \int_{-1}^1 (1-x)^{c\alpha+a} (1+x)^{d\alpha+b} \left| \mathcal{C}_m^{(\alpha)}(x) \right|^\kappa dx \quad (1.27)$$

has the following asymptotics:

$$J_2(a, b, c, d, \kappa, m; \alpha) \sim e^{-\alpha\phi(x_m)} \sqrt{\frac{2\pi}{\alpha}} \frac{2^{\kappa m} ((\alpha)_m)^\kappa}{(m!)^\kappa} \sum_{k=0}^{\infty} \frac{D_k}{\alpha^k}, \quad \alpha \rightarrow \infty \quad (1.28)$$

where the coefficients  $D_k$  do not depend on  $\alpha$ . The first coefficient is given by

$$D_0 = a_1 \left( \frac{2c}{c+d} \right)^a \left( \frac{2d}{c+d} \right)^b \left( \frac{d-c}{c+d} \right)^{\kappa m}, \quad (1.29)$$

and the symbols  $x_m = (d-c)/(d+c)$ ,  $\phi(x_m) = -c \log \frac{2c}{c+d} - d \log \frac{2d}{c+d}$  and  $a_1 = 2\sqrt{\frac{cd}{(c+d)^3}}$ . Moreover, if  $c = d$ , the corresponding Rényi-type functional

$$J_2(a, b, c, \kappa, m; \alpha) = \int_{-1}^1 (1-x)^a (1+x)^b e^{-\alpha\phi(x)} \left| \mathcal{C}_m^{(\alpha)}(x) \right|^\kappa dx, \quad (1.30)$$

has the asymptotic behavior

$$J_2(a, b, c, \kappa, m; \alpha) \sim \sqrt{\frac{\pi}{\alpha c}} \frac{(2\alpha)^m}{m!}, \quad \alpha \rightarrow \infty. \quad (1.31)$$

Finally, the asymptotics of the Rényi-like functional with  $c > d$  follows from the one with  $c < d$  by interchanging  $a$  and  $b$  and  $c$  and  $d$ . The case  $c > d$  is useful for the determination of the Rényi entropy of the high dimensional hydrogenic states in momentum space with  $q < 1$ . For further details about the theorem and its proof, see [123].

### 1.3 Linearization methods of orthogonal polynomials

The linearization problem in the theory of orthogonal polynomials has a long history [46, 51, 55, 125]. It is equivalent to the problem of the evaluation of the integral of the product of three or more orthogonal polynomials of the same kind. A procedure to obtain linearization formulas uses the generating function but it is not hopeful in general. In fact they have been obtained by means of one or more characterizations of the hypergeometric orthogonal polynomials (e.g., orthogonality relation, second-order differential equation, three-term recurrence relations,...) [126? –133] with different success. In this section we briefly describe two scarcely known methods of linearization of natural powers of polynomials: the Srivastava-Niukkanen approach [49, 134] which linearizes the power of an orthogonal polynomial of hypergeometric type (Hermite, Laguerre, Jacobi), and an expansion method [135] of powers of arbitrary polynomials which is based on the Bell polynomials used in combinatorial mathematics [136]. These methods play a predominant role for the analytical determination of the Rényi entropies for both multidimensional hydrogenic and harmonic systems as will be discussed in subsections 2.3 and 3.3, respectively.

#### 1.3.1 Srivastava-Niukkanen approach

The calculation of the integrals containing arbitrary (i.e., non-necessarily integer) powers of a given hypergeometric orthogonal polynomial are relevant from both fundamental and applied standpoints. Indeed, they are closely related to its  $\mathcal{L}_q$  norms (see e.g. [50, 137]) and to different quantifiers of the polynomial spreading all over its orthogonality interval such as the information-theoretic lengths [54, 115, 135, 138] and various entropic quantities of the Rakhmanov probability density of the polynomial. Moreover, they admit combinatorial [46, 133] and entropic [54, 115, 135, 138] interpretations, and they describe the expectation values of some quantum observables of the Hilbert space of numerous physical systems (which are the quantum-mechanical predictions of the experimentally accessible physical quantities) [139].

In this subsection we give two Theorems which provide linearization formulas for the integer  $r$ th-power of Laguerre  $L_n^{(\alpha)}(ty)$  and Jacobi  $P_n^{(\alpha,\beta)}(z)$  polynomials obtained by Sánchez-Moreno et al. [134] using the linearization method of Srivastava-Niukkanen [49]. The associated linearization coefficients are expressed in terms of a multivariate



Lauricella functions  $F_A^{(r+1)}(t, \dots, t, 1)$  and the Srivastava-Daoust generalized function  $F_{1:1;1;\dots;1}^{1:2;\dots;2}(1, \dots, 1)$  for the Laguerre and Jacobi cases, respectively.

**Theorem 1.5.** [49, 134] *The orthogonal Laguerre polynomials  $L_n^{(\alpha)}$ ,  $\alpha > -1$ , satisfy the linearization formula*

$$x^\mu \left[ L_n^{(\alpha)}(tx) \right]^r = \sum_{i=0}^{\infty} c_i(\mu, r, t, n, \alpha, \gamma) L_i^{(\gamma)}(x), \quad (1.32)$$

where  $x \in (0, \infty)$ , the parameters  $\mu \in \mathbb{R}$ ,  $t > 0$ ,  $r \in \mathbb{N}$  and  $\gamma > -1$  is a free parameter, and the linearization coefficients are given by

$$c_i(\mu, r, t, n, \alpha, \gamma) = (\gamma + 1)_\mu \binom{n + \alpha}{n}^r \times F_A^{(r+1)} \left( \begin{array}{c} \gamma + \mu + 1; \overbrace{-n, \dots, -n}^r, -i \\ \alpha + 1, \dots, \alpha + 1, \gamma + 1 \\ \overbrace{\phantom{\alpha + 1, \dots, \alpha + 1, \gamma + 1}}^r \end{array} ; \overbrace{t, \dots, t}^r, 1 \right).$$

The symbol  $F_A^{(s)}$  denotes the Lauricella function of type A of  $s$  variables and  $2s + 1$  parameters is defined [49] as follows:

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

where the symbol  $(y)_z$  denotes the Pochhammer symbol  $(y)_z = \frac{\Gamma(y+z)}{\Gamma(y)}$ . Note that when the number of variables is  $s = 1$ , one recovers the Gauss' hypergeometric function  ${}_2F_1(x)$  [59].

**Theorem 1.6.** [49, 134] *The orthogonal Jacobi polynomials  $P_n^{(\alpha, \beta)}(z)$ ,  $z \in [-1, +1]$ , satisfy the linearization formula*

$$z^\mu \left[ P_n^{(\alpha, \beta)}(z) \right]^r = \sum_{i=0}^{\infty} \tilde{c}_i(\mu, r, n, \alpha, \beta, \gamma, \delta) P_i^{(\gamma, \delta)}(z) \quad (1.33)$$

where  $\alpha, \beta, \gamma, \delta > -1, \mu \in \mathbb{R}, r \in \mathbb{N}$ , and the series coefficients are expressed as

$$\tilde{c}_i(\mu, r, n, \alpha, \beta, \gamma, \delta) = \binom{n+\alpha}{n}^r (\gamma+1)_\mu \frac{(\gamma+\delta+2i+1)(-\mu)_i}{(\gamma+1)_i(\gamma+\delta+i+1)_{\mu+1}}$$

$$\times F_{2:1;\dots;1}^{2:2;\dots;2} \left( \begin{matrix} \mu+1, \gamma+\mu+1 : \overbrace{-n, \alpha+\beta+n+1; \dots, -n, \alpha+\beta+n+1}^r \\ \mu-i+1, \gamma+\delta+\mu+i+2 : \underbrace{\alpha+1, \dots, \alpha+1}_r \end{matrix} ; \overbrace{1, \dots, 1}^r \right).$$

The symbol  $F_{1:1;\dots;1}^{1:2;\dots;2}(1, \dots, 1)$  is a particular instance of the Srivastava-Daoust generalized function  $F_{q_0:q_1;\dots;q_r}^{p_0:p_1;\dots;p_r}(x_1, \dots, x_r)$  which is defined [49] as follows: Given two sets of  $r+1$  integer numbers  $p_0, \dots, p_r$  and  $q_0, \dots, q_r$  and two sets of  $r+1$  real vectors  $\mathbf{a}_i = (a_i^{(1)}, \dots, a_i^{(p_i)})$ ,  $\mathbf{b}_i = (b_i^{(1)}, \dots, b_i^{(q_i)})$  with  $i = 0, \dots, r$ , and taking the notation

$$(\mathbf{a}_i)_j = (a_i^{(1)})_j \cdots (a_i^{(p_i)})_j, \quad (\mathbf{b}_i)_j = (b_i^{(1)})_j \cdots (b_i^{(q_i)})_j,$$

the  $r$ -variate Srivastava-Daoust function of  $r$  variables  $(x_1, \dots, x_r)$  and  $N = \sum_{i=0}^r (p_i + q_i)$  real parameters, is defined as

$$F_{q_0:q_1;\dots;q_r}^{p_0:p_1;\dots;p_r} \left( \begin{matrix} \mathbf{a}_0 : \mathbf{a}_1; \dots; \mathbf{a}_r, \\ \mathbf{b}_0 : \mathbf{b}_1; \dots; \mathbf{b}_r \end{matrix} ; x_1, \dots, x_r \right) = \sum_{j_1, \dots, j_r=0}^{\infty} \left( \prod_{i=0}^r \frac{(\mathbf{a}_i)_{j_i}}{(\mathbf{b}_i)_{j_i}} \frac{x_i^{j_i}}{j_i!} \right), \quad (1.34)$$

where  $j_0 \equiv j_1 + j_2 + \dots + j_r$ , and  $\frac{x_0^{j_0}}{j_0!} \equiv 1$  is understood.

These two theorems will be used to carry out the computation of the exact Rényi entropies for both hydrogenic (see Sec. 2.3) and harmonic states (see Secs. 3.1 and 3.3).

### 1.3.2 Bell-polynomial-based method

In this subsection we give a Lemma which provides an expansion method of powers of arbitrary polynomials in which the expansion coefficients are given by means of the multivariate Bell polynomials of combinatorial mathematics [136]. This method has been recently used [54, 135, 138] to obtain a number of entropy-like integral functionals of the hypergeometric orthogonal polynomials.

#### Definition 1.7. Bell polynomials

Given natural numbers  $n \geq k$ , the Bell polynomial of the second kind with  $n-k+1$  variables is defined as

$$B_{n,k}(x_1, x_2, \dots, x_{n-k+1}) = \sum_{j_1, \dots, j_{n-k+1}} \frac{n!}{j_1! \cdots j_{n-k+1}!} \left( \frac{x_1}{1!} \right)^{j_1} \cdots \left( \frac{x_{n-k+1}}{(n-k+1)!} \right)^{j_{n-k+1}}$$

where the sum indices are restricted for the following relations  $j_1 + j_2 + \cdots + j_{n-k+1} = k$  and  $j_1 + 2j_2 + \cdots + (n - k + 1)j_{n-k+1} = n$ .

**Lemma 1.8.** [135] *The  $p$ -th power of a given polynomial  $y_n(x) = \sum_{k=0}^n c_k x^k$  can be expressed as*

$$(y_n(x))^p = \sum_{k=0}^{np} A_{k,p}(c_0, \dots, c_n) x^k \quad (1.35)$$

with

$$A_{k,p}(c_0, \dots, c_n) = \frac{p!}{(p+k)!} B_{p+k,p}(c_0, 2!c_1, \dots, (k+1)!c_k) \quad (1.36)$$

$$= \sum_{j_1, \dots, j_n} \frac{p!}{j_0! j_1! \cdots j_n!} c_0^{j_0} c_1^{j_1} \cdots c_n^{j_n} \quad (1.37)$$

where the sum indices are restricted for the following relations  $j_1 + j_2 + \cdots + j_n = p$  and  $j_1 + 2j_2 + \cdots + nj_n = k$ .

This method will be used later in this work (Sec. 3.1) for the determination of the angular part of the physical Rényi entropies of the three-dimensional quantum harmonic systems [64].

## Chapter 2

# Rényi and Shannon entropies of Coulomb systems

The goal of this chapter is to investigate the internal disorder of the  $D$ -dimensional Coulomb systems of hydrogenic type by means of the analytical information theory. This includes the quantification of the multiple facets of the multi-dimensional geometries of the charge and momentum probability distributions of the discrete stationary quantum-mechanical states of the systems by means of their associated Rényi and Shannon entropies.

The analytical determination of the Rényi and Shannon entropies of the main prototype of the  $D$ -dimensional Coulomb many-body systems, the  $D$ -dimensional hydrogenic system, from first principles (i.e., in terms of the hyperquantum numbers of the state and the nuclear charge) has been recently undertaken [31, 41, 74, 140]. This is relevant *per se* and for a reference point of view. The  $D$ -dimensional hydrogenic system is a negatively-charged particle moving in a space of  $D$  dimensions around a positively charged core which electromagnetically binds it in its orbit [37, 41, 57, 141, 142]. This system allows for the modelling of numerous three-dimensional physical systems (e.g., hydrogenic atoms and ions, exotic atoms, antimatter atoms, Rydberg atoms) and a number of nanotechnological objects (quantum wells, wires and dots) and qubits which have been shown to be very useful in semiconductor physics [143, 144] and quantum technologies [145, 146], respectively. Moreover, it plays a crucial role for the interpretation of numerous phenomena of quantum cosmology and quantum field theory [147, 148]. In addition the  $D$ -dimensional hydrogenic wavefunctions have been used as complete orthonormal sets for many-body atomic and molecular problems [57, 58] in both position and momentum spaces.

The calculation of the hydrogenic Rényi and Shannon entropies is a formidable task except for the lowest-lying energy states. This is because these quantities are described

by means of some power and logarithmic functionals of the electron density, respectively, which cannot be easily handled in an analytical way nor numerically computed. The latter is basically because a naive numerical evaluation using quadratures is not convenient due to the increasing number of integrable singularities when the principal hyperquantum number  $n$  is increasing, which spoils any attempt to achieve reasonable accuracy even for rather small  $n$  [149].

Up until now, these quantities have been only calculated for the standard (three-dimensional) hydrogenic system in a closed form [31, 140] at the high-energy (Rydberg) limit. In this Chapter we extend this achievement for the Rydberg and the pseudo-classical states of  $D$ -dimensional hydrogenic systems [31, 63] by use of modern asymptotical techniques [122, 123] of the Laguerre and Gegenbauer polynomials which control the state's wavefunctions in position and momentum spaces. Furthermore we obtain the Rényi entropies for all discrete stationary states of the standard and non-standard multidimensional hydrogenic systems [70] by means of the linearization techniques of orthogonal polynomials described in the previous chapter.

This chapter is composed by three sections. Shortly, the main results of each section are the following:

- 2.1 We determine the three main entropic measures (Rényi, Shannon, Tsallis) of the quantum probability density of the  $D$ -dimensional Rydberg hydrogenic states in terms of the basic parameters which characterize them; namely, the dimensionality  $D$ , the hyperquantum numbers  $(n, l, \{\mu\})$  and the nuclear charge  $Z$  of the system. The Theorem of Aptekarev et al discussed in Chapter 1, which gives the asymptotics of the entropy-like integral functionals of Laguerre polynomials, has been used.
- 2.2 We calculate the high- $D$  behavior of the position and momentum Rényi entropies of the  $D$ -dimensional hydrogenic states in terms of the state's hyperquantum numbers and the nuclear charge  $Z$  of the system. We have used a recent constructive methodology based on Temme et al's Theorem (see Chapter 1) which allows for the calculation of some Rényi-like integral functionals of Laguerre  $\mathcal{L}_k^{(\alpha)}(x)$  and Gegenbauer  $\mathcal{C}_k^{(\alpha)}(x)$  polynomials with a fixed degree  $k$  and large values of the parameter  $\alpha$ .
- 2.3 We obtain the position  $R_q[\rho_{n,l,\{\mu\}}]$  and momentum  $R_q[\gamma_{n,l,\{\mu\}}]$  Rényi entropies (with integer  $q$  greater than 1) for all the multidimensional hydrogenic states in terms of the Rényi parameter,  $q$ , the spatial dimension  $D$ , the nuclear charge  $Z$  as well as the hyperquantum numbers,  $(n, l, \{\mu\})$ , which characterize the corresponding wavefunction of the states. The linearization and expansion techniques of Laguerre and Jacobi polynomials described in Chapter 1 have been used.

## 2.1 Rydberg states

Coulomb systems at Rydberg states are huge-size atoms which can be made by exciting the outermost electron in certain elements, so that all the inner electrons can be lumped together and regarded, along with the atom's nucleus, as a unified core, with the lone remaining electron lying outside. Thus, they are as if the atom were a hydrogenic system, a heavy version of hydrogen. Due to their extraordinary properties (high magnetic susceptibility, relatively long lifetime, high kinetic energy, ...) these systems, where the outermost electrons are highly excited but not ionized, have been used in multiple scientific areas ranging from plasmas and diamagnetism to astrophysics, quantum chaos and strongly interacting systems. Recently it has been argued that they might be just the basic elements for processing quantum information (see e.g., [150, 151]). Indeed, these oversized atoms can be sustained for a long time in a quantum superposition condition (what is very convenient for creating qubits) and they can interact strongly with other such atoms; this property makes them very useful for devising the kind of logic gates needed to process information.

The multidimensional Rydberg hydrogenic states (i.e. states where the electron has a large principal hyperquantum number  $n$ , so being highly excited), with standard and non-standard dimensionalities, has been investigated (see section 5 of [41], and [48, 54, 113, 152]) up until now by means of the following spreading measures: central moments, variances, logarithmic expectation values, Shannon entropy and Fisher information. In this Section we go much beyond this study by calculating the Rényi and Tsallis entropic measures of the highly excited or Rydberg states of the  $D$ -dimensional hydrogenic systems in terms of the principal and orbital hyperquantum numbers and the space dimensionality  $D$ . This has been possible through the use of the novel mathematical technique developed by Aptekarev et al. [122] which has been briefly described in the Sec. 1.2.1.

Precisely, we have carried out the following tasks:

- The Rényi entropy has been calculated by first decomposing it into two parts of radial and angular types, and realizing that the angular part does not depend on  $n$ , so that the true problem to be solved is the calculation of the radial Rényi entropy in the limit of large  $n$ .
- The radial Rényi entropy has been shown to be expressed in terms of the  $\mathfrak{L}_p$ -norms of the Laguerre polynomials which control the Rydberg states we are interested in.
- The remaining asymptotics of these Laguerre norms is determined by means of a recent asymptotical technique of approximation theory given by Theorem 1.1 of Aptekarev et al [122].

- We numerically apply this theoretical methodology to some particular Rydberg hydrogenic states of  $s$  and  $p$  types.
- We find that the Rényi entropy monotonically decreases (increases) when the nuclear charge (the dimensionality) is decreasing (increasing) for some  $s$  and  $p$  states.
- The Shannon and Tsallis entropies can be obtained from the Rényi one.

These results have been published in the article [31] with coordinates: Toranzo I. V., **Puertas-Centeno D.** and Dehesa J. S. *Entropic properties of  $D$ -dimensional Rydberg systems*. Physica A: Statistical Mechanics and its Applications, 462:1197-1206, 2016, which is attached below.

# Entropic properties of $D$ -dimensional Rydberg systems

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The fundamental information-theoretic measures (the Rényi  $R_p[\rho]$  and Tsallis  $T_p[\rho]$  entropies,  $p > 0$ ) of the highly-excited (Rydberg) quantum states of the  $D$ -dimensional ( $D > 1$ ) hydrogenic systems, which include the Shannon entropy ( $p \rightarrow 1$ ) and the disequilibrium ( $p = 2$ ), are analytically determined by use of the strong asymptotics of the Laguerre orthogonal polynomials which control the wavefunctions of these states. We first realize that these quantities are derived from the entropic moments of the quantum-mechanical probability  $\rho(\vec{r})$  densities associated to the Rydberg hydrogenic wavefunctions  $\Psi_{n,l,\{\mu\}}(\vec{r})$ , which are closely connected to the  $\mathcal{L}_p$ -norms of the associated Laguerre polynomials. Then, we determine the ( $n \rightarrow \infty$ )-asymptotics of these norms in terms of the basic parameters of our system (the dimensionality  $D$ , the nuclear charge and the hyperquantum numbers  $(n, l, \{\mu\})$  of the state) by use of recent techniques of approximation theory. Finally, these three entropic quantities are analytically and numerically discussed in terms of the basic parameters of the system for various particular states.

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## I. INTRODUCTION

Rydberg systems are ballooned-up atoms which can be made by exciting the outermost electron in certain elements, so that all the inner electrons can be lumped together and regarded, along with the atom's nucleus, as a unified core, with the lone remaining electron lying outside [1, 2]. Thus, they are as if the atom were a hydrogenic system, a heavy version of hydrogen. Due to their extraordinary properties (high magnetic susceptibility, relatively long lifetime, high kinetic

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energy,...) these systems, where the outermost electrons are highly excited but not ionized, have been used in multiple scientific areas ranging from plasmas and diamagnetism to astrophysics, quantum chaos and strongly interacting systems. Recently it has been argued that they might be just the basic elements for processing quantum information (see e.g., [3, 4]). Indeed, these outsized atoms can be sustained for a long time in a quantum superposition condition (what is very convenient for creating qubits) and they can interact strongly with other such atoms; this property makes them very useful for devising the kind of logic gates needed to process information.

The  $D$ -dimensional hydrogenic system (i.e. an electron or a negatively-charged particle moving around a nucleus or a positively-charged core which electromagnetically binds it in its orbit), with  $D > 1$ , is the main prototype to model the behavior of most multidimensional quantum many-body systems with standard ( $D = 3$ ) and non-standard ( $D \neq 3$ ) dimensionalities [5–10]. It embraces a large variety of three-dimensional physical systems (e.g., hydrogenic atoms and ions, exotic atoms, antimatter atoms, Rydberg atoms,...) and a number of nanotechnological objects which have been shown to be very useful in semiconductor nanostructures (e.g., quantum wells, wires and dots) [11, 12] and quantum computation (e.g., qubits) [13, 14]. Moreover, it plays a crucial role for the interpretation of numerous phenomena of quantum cosmology [15] and quantum field theory [5, 16, 17]. As well, the  $D$ -dimensional hydrogenic wavefunctions have been used as complete orthonormal sets for many-body atomic and molecular problems [18–20] in both position and momentum spaces. Finally, the existence of non-standard hydrogenic systems has been proved for  $D < 3$  [12, 21] and suggested for  $D > 3$  [7].

The multidimensional extension of Rydberg hydrogenic states (i.e. states where the electron has a large principal quantum number  $n$ , so being highly excited), with standard and non-standard dimensionalities, has been investigated (see section 5 of [22], and [23–26]) up until now by means of the following spreading measures: central moments, variances, logarithmic expectation values, Shannon entropy and Fisher information. These measures were found to be expressed in terms of the principal and orbital hyperquantum numbers and the space dimensionality  $D$ . In this work we go much beyond this study by calculating the Rényi [27] and Tsallis [28] entropies (also called by *information generating functionals* [29]) of the Rydberg states defined by

$$R_p[\rho] = \frac{1}{1-p} \ln W_p[\rho]; \quad 0 < p < \infty, \quad (1)$$

$$T_p[\rho] = \frac{1}{p-1} (1 - W_p[\rho]); \quad 0 < p < \infty, \quad (2)$$

where the symbol  $W_p[\rho]$  denotes the entropic moments of  $\rho(\vec{r})$  defined as

$$W_p[\rho] = \int_{\mathbb{R}^D} [\rho(\vec{r})]^p d\vec{r} = \|\rho\|_p^p; \quad p > 0. \quad (3)$$

The symbol  $\|\cdot\|_p$  denotes the  $\mathfrak{L}_p$ -norm for functions:  $\|\Phi\|_p = (\int_{\mathbb{R}^D} |\Phi(\vec{r})|^p d\vec{r})^{1/p}$ . Note that both Rényi and Tsallis measures include the Shannon entropy,  $S[\rho] = \lim_{p \rightarrow 1} R_p[\rho] = \lim_{p \rightarrow 1} T_p[\rho]$ , and the disequilibrium,  $\langle \rho \rangle = \exp(R_2[\rho])$ , as two important particular cases. Moreover, they are interconnected as indicated later on. Their properties have been recently reviewed [25, 30, 31]; see also [32–37]. Moreover, the Rényi entropies and their associated uncertainty relations have been widely used to investigate a great deal of quantum-mechanical properties and phenomena of physical systems and processes [25, 30, 38], ranging from the quantum-classical correspondence [39] and quantum entanglement [40] to pattern formation and Brown processes [41, 42], quantum phase transition [43] and disordered systems [44].

The structure of this work is the following. First, in Section II, we give the wavefunctions of the stationary  $D$ -dimensional hydrogenic states in position space and their squares, the quantum probability densities  $\rho(\vec{r})$ . Then we define the entropic moments and the Rényi entropy of this density, and we show that for the very excited states the calculation of the latter quantity essentially converts into the determination of the asymptotics of the  $\mathfrak{L}_p$ -norm of the Laguerre polynomials which control the states' wavefunctions. In Section III we use a powerful technique of approximation theory recently developed by Aptekarev et al [26, 45, 46] to determine these Laguerre norms in terms of  $D$  and the hyperquantum numbers of the system. In Section IV the Shannon, Rényi and Tsallis entropies are studied both analytically and numerically for the  $D$ -dimensional hydrogenic states by means of  $D$ , the hyperquantum numbers and the nuclear charge  $Z$  of the system. Finally, some concluding remarks are given.

## II. THE $D$ -DIMENSIONAL RYDBERG PROBLEM: ENTROPIC FORMULATION

In this section we briefly describe the quantum probability density of the stationary states of the  $D$ -dimensional hydrogenic system in position space. Then, we pose the determination of the entropic moments and the Rényi entropies of this density in the most appropriate mathematical manner for our purposes. Atomic units will be used throughout.

The time-independent Schrödinger equation of a  $D$ -dimensional ( $D \geq 1$ ) hydrogenic system (i.e., an electron moving under the action of the  $D$ -dimensional Coulomb potential  $V(\vec{r}) = -\frac{Z}{r}$ ) is given

by

$$\left(-\frac{1}{2}\vec{\nabla}_D^2 - \frac{Z}{r}\right)\Psi(\vec{r}) = E\Psi(\vec{r}), \quad (4)$$

where  $\vec{\nabla}_D$  denotes the  $D$ -dimensional gradient operator,  $Z$  is the nuclear charge, and the electronic position vector  $\vec{r} = (x_1, \dots, x_D)$  in hyperspherical units is given as  $(r, \theta_1, \theta_2, \dots, \theta_{D-1}) \equiv (r, \Omega_{D-1})$ ,  $\Omega_{D-1} \in S^{D-1}$ , where  $r \equiv |\vec{r}| = \sqrt{\sum_{i=1}^D x_i^2} \in [0; +\infty)$  and  $x_i = r \left(\prod_{k=1}^{i-1} \sin \theta_k\right) \cos \theta_i$  for  $1 \leq i \leq D$  and with  $\theta_i \in [0; \pi)$ ,  $i < D-1$ ,  $\theta_{D-1} \equiv \phi \in [0; 2\pi)$ . It is assumed that the nucleus is located at the origin and, by convention,  $\theta_D = 0$  and the empty product is the unity. .

It is known [16, 22, 47, 48] that the energies belonging to the discrete spectrum are given by

$$E = -\frac{Z^2}{2\eta^2}, \quad \eta = n + \frac{D-3}{2}; \quad n = 1, 2, 3, \dots, \quad (5)$$

and the associated eigenfunction can be expressed as

$$\Psi_{\eta, l, \{\mu\}}(\vec{r}) = \mathcal{R}_{\eta, l}(r) \mathcal{Y}_{l, \{\mu\}}(\Omega_{D-1}). \quad (6)$$

Then, the quantum probability density of a  $D$ -dimensional hydrogenic stationary state  $(n, l, \{\mu\})$  is given by the squared modulus of the position eigenfunction as

$$\rho_{n, l, \{\mu\}}(\vec{r}) = \rho_{n, l}(\tilde{r}) |\mathcal{Y}_{l, \{\mu\}}(\Omega_{D-1})|^2, \quad (7)$$

where the radial part of the density is the univariate function

$$\rho_{n, l}(\tilde{r}) = [\mathcal{R}_{n, l}(r)]^2 = \frac{\lambda^{-d}}{2\eta} \frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{d-2}} [\widehat{\mathcal{L}}_{\eta-L-1}^{(2L+1)}(\tilde{r})]^2 \quad (8)$$

with  $L$ , defined as the ‘‘grand orbital angular momentum quantum number’’, and the adimensional parameter  $\tilde{r}$  given by

$$L = l + \frac{D-3}{2}, \quad l = 0, 1, 2, \dots \quad (9)$$

$$\tilde{r} = \frac{r}{\lambda}, \quad \lambda = \frac{\eta}{2Z}. \quad (10)$$

The symbols  $\mathcal{L}_n^{(\alpha)}(x)$  and  $\widehat{\mathcal{L}}_n^{(\alpha)}(x)$  denote the orthogonal and orthonormal, respectively, Laguerre polynomials with respect to the weight  $\omega_\alpha(x) = x^\alpha e^{-x}$  on the interval  $[0, \infty)$ , so that

$$\widehat{\mathcal{L}}_m^{(\alpha)}(x) = \left(\frac{m!}{\Gamma(m+\alpha+1)}\right)^{1/2} \mathcal{L}_m^{(\alpha)}(x), \quad (11)$$

and finally

$$K_{\eta, L} = \lambda^{-\frac{D}{2}} \left\{ \frac{(\eta-L-1)!}{2\eta(\eta+L)!} \right\}^{\frac{1}{2}} = \left\{ \left( \frac{2Z}{n + \frac{D-3}{2}} \right)^D \frac{(n-l-1)!}{2 \left( n + \frac{D-3}{2} \right) (n+l+D-3)!} \right\}^{\frac{1}{2}} \equiv K_{n, l} \quad (12)$$

represents the normalization constant which ensures that  $\int |\Psi_{\eta,l,\{\mu\}}(\vec{r})|^2 d\vec{r} = 1$ . The angular eigenfunctions are the hyperspherical harmonics,  $\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})$ , defined as

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

with the normalization constant

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

where the symbol  $C_n^\lambda(t)$  denotes the Gegenbauer polynomial of degree  $n$  and parameter  $\lambda$ .

Now we can calculate any spreading measure of the  $D$ -dimensional hydrogenic system beyond the known the variance and the ordinary moments (or radial expectation values) of its density, which are already known [22]. The most relevant spreading quantities are the entropic moments  $W_p[\rho_{n,l,\{\mu\}}]$ , because they characterize the density and moreover we can obtain from them the main entropic measures of the system such as the Rényi, Shannon and Tsallis entropies. They are given as

$$\begin{aligned} W_p[\rho_{n,l,\{\mu\}}] &= \int_{\mathbb{R}^D} [\rho_{n,l,\{\mu\}}(\vec{r})]^p d\vec{r} \\ &= \int_0^\infty [\rho_{n,l}(r)]^p r^{D-1} dr \times \Lambda_{l,\{\mu\}}(\Omega_{D-1}), \end{aligned} \quad (13)$$

where we have used that the volume element is

$$d\vec{r} = r^{D-1} dr d\Omega_{D-1}, \quad d\Omega_{D-1} = \left( \prod_{j=1}^{D-2} \sin^{2\alpha_j} \theta_j \right) d\phi,$$

(with  $2\alpha_j = D - j - 1$ ) and the angular part is given by

$$\Lambda_{l,\{\mu\}}(\Omega_{D-1}) = \int_{S^{D-1}} |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^{2p} d\Omega_{D-1}. \quad (14)$$

Then, from Eqs. (1) and (13) we can obtain the Rényi entropies of the  $D$ -dimensional hydrogenic state  $(n, l, \{\mu\})$  as follows

$$R_p[\rho_{n,l,\{\mu\}}] = R_p[\rho_{n,l}] + R_p[\mathcal{Y}_{l,\{\mu\}}], \quad (15)$$

where  $R_p[\rho_{n,l}]$  denotes the radial part

$$R_p[\rho_{n,l}] = \frac{1}{1-p} \ln \int_0^\infty [\rho_{n,l}]^p r^{D-1} dr, \quad (16)$$

and  $R_p[\mathcal{Y}_{l,\{\mu\}}]$  denotes the angular part

$$R_p[\mathcal{Y}_{l,\{\mu\}}] = \frac{1}{1-p} \ln \Lambda_{l,\{\mu\}}(\Omega_{D-1}). \quad (17)$$

In this work we are interested in the entropic properties of the high extreme region of the system, embracing the highly and very highly excited (Rydberg) states (recently shown to be experimentally accessible [1]) where these properties are most difficult to compute because they possess large and very large values of  $n$ . Since the dependence of both the entropic moments and the Rényi entropies on the principal hyperquantum number  $n$  is concentrated in their radial parts according to Eqs. (13)-(17), the computation of  $R_p[\rho_{n,l,\{\mu\}}]$  for the Rydberg states of  $D$ -dimensional hydrogenic systems practically reduces to determine the value of the radial Rényi entropy,  $R_p[\rho_{n,l}]$ , in the limiting case  $n \rightarrow \infty$ . Moreover, by taking into account the expression (8) of the radial density and Eqs. (13) and (16), this problem converts into the study of the asymptotics ( $n \rightarrow \infty$ ) of the  $\mathfrak{L}_p$ -norm of the Laguerre polynomials

$$N_n(\alpha, p, \beta) = \int_0^\infty \left( \left[ \widehat{\mathcal{L}}_n^{(\alpha)}(x) \right]^2 w_\alpha(x) \right)^p x^\beta dx, \quad \alpha > -1, p > 0, \beta + p\alpha > -1. \quad (18)$$

Indeed, from Eq. (16) one has that the radial Rényi entropy can be expressed as

$$R_p[\rho_{n,l}] = \frac{1}{1-p} \ln \left[ \frac{\eta^{D(1-p)-p}}{2^{D(1-p)+p} Z^{D(1-p)}} N_{n,l}(D, p) \right], \quad (19)$$

where the norm  $N_{n,l}(\alpha, p, \beta) \equiv N_{n,l}(D, p)$  is given by

$$N_{n,l}(D, p) = \int_0^\infty \left( \left[ \widehat{\mathcal{L}}_{n-l-1}^{(\alpha)}(x) \right]^2 w_\alpha(x) \right)^p x^\beta dx, \quad (20)$$

with

$$\alpha = 2L + 1 = 2l + D - 2, \quad l = 0, 1, 2, \dots, n-1, \quad p > 0 \quad \text{and} \quad \beta = (2-D)p + D - 1 \quad (21)$$

We note that (21) guarantees the convergence of integral (20); i.e. the condition  $\beta + p\alpha = 2lp + D - 1 > -1$  is always satisfied for physically meaningful values of the parameters.

### III. LAGUERRE $\mathfrak{L}_p$ -NORMS AND RADIAL ENTROPIES: ASYMPTOTICS

Let us now study the asymptotics at large  $n$  of the Laguerre hydrogenic norms  $N_{n,l}(D, p)$  given by Eq. (20) in terms of all possible values of the involved parameters  $(D, p)$ . It controls

the asymptotic values of the radial Rényi entropy  $R_p[\rho_{n,l}]$  given by Eq. (19) and, because of Eq. (15), the total Rényi entropy of the Rydberg  $D$ -dimensional hydrogenic states. Since the exact evaluation of these norm-like functionals is a very difficult task, not yet solved, we will tackle this problem by means of the determination of the asymptotical behavior (i.e., at large  $n$ ) of the general functional  $N_n(\alpha, p, \beta)$  by extensive use of the strong asymptotics of Laguerre polynomials. The results obtained are contained in the following theorem.

**Theorem.** The asymptotics ( $n \rightarrow \infty$ ) of the Laguerre hydrogenic functionals  $N_{n,l}(D, p)$  defined by Eq. (20) are given by the following expressions for all possible values of  $D$  and  $p > 0$ :

1. If  $\beta > 0$ , there are two subcases:

(a) If  $D > 2$ , then

$$N_{n,l}(D, p) = C(\beta, p) (2(n-l-1))^{1+\beta-p} (1 + \bar{o}(1)), \text{ for } p \in \left(0, \frac{D-1}{D-2}\right) \quad (22)$$

(b) If  $D = 2$  (so,  $\beta = 1$ ), then

$$N_{n,l}(D, p) = \begin{cases} C(1, p) (2(n-l-1))^{2-p} (1 + \bar{o}(1)) , & p \in (0, 2) \\ \frac{\ln(n-l-1) + \underline{O}(1)}{\pi^2} , & p = 2 \text{ (Cosine-Airy regime)} \\ \frac{C_A(p)}{\pi^p} (4(n-l-1))^{\frac{2}{3}(2-p)} (1 + \bar{o}(1)) & p \in (2, 5) \\ \left( \frac{C_A(p)}{\pi^p 4^2} + C_B(\alpha, 1, p) \right) (n-l-1)^{-2}, & p = 5 \\ C_B(\alpha, 1, p) (n-l-1)^{-2} , & p \in (5, \infty). \end{cases} \quad (23)$$

2. If  $\beta = 0$  (so,  $D \neq 2$  and  $p = \frac{D-1}{D-2}$ ), then

$$N_{n,l}(D,p) = \begin{cases} C(0,p) (2(n-l-1))^{(1-p)} (1 + \bar{o}(1)), & p = \frac{D-1}{D-2} \\ \frac{\ln(n-l-1) + \underline{O}(1)}{\pi^2(n-l-1)}, & p = 2, (D=3) \text{ (Cosine-Airy regime)}. \end{cases} \quad (24)$$

3. If  $\beta < 0$  (so, either  $p < \frac{D-1}{D-2}$  and  $D < 2$  or  $p > \frac{D-1}{D-2}$  and  $D > 2$ ), then

$$N_{n,l}(D,p) = \begin{cases} C(\beta,p) (2(n-l-1))^{1+\beta-p} (1 + \bar{o}(1)), & p \in \left(\frac{D-1}{D-2}, \frac{2D}{2D-3}\right) \\ \frac{2\Gamma(p+1/2) (\ln n + \underline{O}(1))}{\pi^{p+1/2} \Gamma(p+1) (4(n-l-1))^{1+\beta}}, & p = 2 + 2\beta = \frac{2D}{2D-3} \text{ (Cosine-Bessel regime)}, \\ C_B(\alpha,\beta,p) (n-l-1)^{-(1+\beta)} (1 + \bar{o}(1)), & p > 2 + 2\beta = \frac{2D}{2D-3} \end{cases} \quad (25)$$

where the constants  $C, C_B, C_A$  are given by

$$C(\beta,p) := \frac{2^{\beta+1}}{\pi^{p+1/2}} \frac{\Gamma(\beta+1-p/2) \Gamma(1-p/2) \Gamma(p+1/2)}{\Gamma(\beta+2-p) \Gamma(1+p)}, \quad (26)$$

$$C_A(p) := \int_{-\infty}^{+\infty} \left[ \frac{2\pi}{\sqrt[3]{2}} \text{Ai}^2 \left( -\frac{t\sqrt[3]{2}}{2} \right) \right]^p dt, \quad (27)$$

and

$$C_B(\alpha,\beta,p) := 2 \int_0^{\infty} t^{2\beta+1} |J_{\alpha}|^{2p}(2t) dt, \quad (28)$$

respectively,  $\alpha = 2l + D - 2$  and  $\beta = (2 - D)p + D - 1$ . The symbols  $Ai(t)$  and  $J_{\alpha}(z)$  denote the Airy and the Bessel functions (see [49]) defined by

$$Ai(y) = \frac{\sqrt[3]{3}}{\pi} A(-3\sqrt{3}y), \quad A(t) = \frac{\pi}{3} \sqrt{\frac{t}{3}} \left[ J_{-1/3} \left( 2 \left( \frac{t}{3} \right)^{\frac{3}{2}} \right) + J_{1/3} \left( 2 \left( \frac{t}{3} \right)^{\frac{3}{2}} \right) \right].$$

and

$$J_{\alpha}(z) = \sum_{\nu=0}^{\infty} \frac{(-1)^{\nu}}{\nu! \Gamma(\nu + \alpha + 1)} \left( \frac{z}{2} \right)^{\alpha+2\nu}.$$

respectively.

*Comment:* For  $D = 3$  it happens that  $\frac{2D}{2D-3} = \frac{D-1}{D-2} = 2$ , and then the quantities  $N_{n,l}(D, p)$  are given by the third asymptotical expression in (25). For higher dimensions one has  $\frac{2D}{2D-3} > \frac{D-1}{D-2}$ , and the three expressions in (25) hold.

*Hints.* We use the effective Aptekarev et al's technique [26, 45, 46] recently applied for oscillator-like systems. This technique determines the  $(n \rightarrow \infty)$ -asymptotics of the Laguerre hydrogenic norms  $N_n(\alpha, p, \beta)$  by taking care of the values of the parameters  $\alpha, \beta$  and  $p$ . It turns out that the dominant contribution to the asymptotical value of the integral (18) comes from different regions of integration defined according to the values of the involved parameters, which characterize various asymptotic regimes. Thus, we have to use various asymptotical representations for the Laguerre polynomials at the different scales.

Altogether there are five asymptotical regimes which can give (depending on  $\alpha, \beta$  and  $p$ ) the dominant contribution in the asymptotics of  $N_n(\alpha, p, \beta)$ . Three of them exhibit the growth of  $N_n(\alpha, p, \beta)$  as some  $n$ th-power law with an exponent which depends on  $\alpha, \beta$  and  $p$ . We call them by Bessel, Airy and cosine (or oscillatory) regimes, which are characterized by the constants  $C_B, C_A$  and  $C$ , respectively, mentioned above. The Bessel regime corresponds to the neighborhood of zero (i.e. the left end point of the interval of orthogonality), where the Laguerre polynomials can asymptotically be expressed by means of Bessel functions (taken for expanding scale of the variable). Then, at the right of zero (cosine regime) the oscillatory behavior of the polynomials (in the bulk region of zeros location) is modeled asymptotically by means of the trigonometric functions; and at the neighborhood of the extreme right of zeros (Airy regime) the asymptotics of the Laguerre polynomials is controlled by Airy functions. Finally, in the neighborhood of the infinity point of the orthogonality interval the polynomials have growing asymptotics. Moreover, there are regions where these asymptotics match each other. Namely, asymptotics of the Bessel functions for big arguments match the trigonometric function, as well as the asymptotics of the Airy functions do the same.

In addition, there are two transition regimes: cosine-Bessel and cosine-Airy. If the contributions of these regimes dominate in the integral (18), then the asymptotics of  $N_n(\alpha, p, \beta)$  besides the degree on  $n$  have the factor  $\ln n$ . Note also that if these regimes dominate, then the gamma factors in constant  $C(\beta, p)$  in (26) for the oscillatory cosine regime blow up. For the cosine-Bessel regime this happens when  $\beta + 1 - p/2 = 0$ , and for the cosine-Airy regime when  $1 - p/2 = 0$ .



#### IV. INFORMATION ENTROPIES OF THE $D$ -DIMENSIONAL RYDBERG STATES

In this section we determine the Rényi, Shannon and Tsallis entropies of the  $D$ -dimensional Rydberg hydrogenic states in terms of the spatial dimension  $D$ , the order parameter  $p$ , the hyper-quantum numbers  $(n, l, \{\mu\})$  and the nuclear charge  $Z$ . First, attention is focussed on the Rényi and Shannon entropies since the Tsallis entropy can be obtained from the Rényi one by means of the relation

$$T_p[\rho] = \frac{1}{1-p} [e^{(1-p)R_p[\rho]} - 1]. \quad (29)$$

Then, for illustration, we numerically discuss the Rényi entropy  $R_p[\rho_{n,0,0}]$  of some hydrogenic Rydberg ( $ns$ )-states in terms of  $D$ ,  $p$ ,  $n$  and  $Z$ .

Let us start by pointing out that the total Rényi entropy  $R_p[\rho_{n,l,\{\mu\}}]$  of the Rydberg states can be obtained in a straightforward manner by taking into account Eq. (15), the values of the radial Rényi entropy  $R_p[\rho_{n,l}]$  derived from Eq. (19), the asymptotical ( $n \rightarrow \infty$ ) values of the Laguerre norms  $N_{n,l}(D, p)$  given by the previous theorem, and the angular Rényi entropy  $R_p[\mathcal{Y}_{l,\{\mu\}}]$  given by Eqs. (14) and (17); keep in mind that the angular part of the Rényi entropy does not depend on the principal quantum number  $n$ .

What about the Shannon entropy  $S[\rho_{n,l,\{\mu\}}]$  of the Rydberg hydrogenic states?. To calculate its value for any stationary state  $(n, l, \{\mu\})$ , we take into account (a) that  $\lim_{p \rightarrow +1} R_p[\rho] = S[\rho]$  for any probability density  $\rho$ , (b) the expression (15), (c) the following limiting value of the radial Rényi entropy  $R_p[\rho_{n,l,\{\mu\}}]$  of the Rydberg hydrogenic states obtained for a fixed dimension  $D$  from (19)-(20) and the previous theorem,

$$\begin{aligned} \lim_{p \rightarrow +1} R_p[\rho_{n,l}] &= \lim_{p \rightarrow +1} \frac{1}{1-p} \ln \left[ \frac{\eta^{D(1-p)-p}}{2^{D(1-p)+p} Z^{D(1-p)}} C(\beta, p) (2n)^{1+\beta-p} \right] \\ &= 2D \ln n + (2-D) \ln 2 + \ln \pi - D \ln Z + D - 3, \end{aligned} \quad (30)$$

(d) the condition  $n \gg l$  and (e) that

$$\lim_{p \rightarrow +1} R_p[\mathcal{Y}_{l,\{\mu\}}] = \lim_{p \rightarrow +1} \frac{1}{1-p} \ln \Lambda_{l,m}(\Omega_{D-1}) = S[\mathcal{Y}_{l,\{\mu\}}], \quad (31)$$

(remember (14) and (15) for the first equality) where  $S[\mathcal{Y}_{l,\{\mu\}}]$  is the Shannon-entropy functional of the spherical harmonics [50] given by

$$S[\mathcal{Y}_{l,\{\mu\}}] = - \int_{S^{D-1}} [\mathcal{Y}_{l,\{\mu\}}]^2 \ln [\mathcal{Y}_{l,\{\mu\}}]^2 d\Omega_{D-1}. \quad (32)$$

which does not depend on  $n$  and can be calculated as indicated in [24]. In particular, from the previous indications we find the following values

$$R_p[\rho_{n,0,0}] = R_p[\rho_{n,0}] + R_p[\mathcal{Y}_{0,0}] = R_p[\rho_{n,0}] + \frac{1}{1-p} \ln f(p, D) \quad (33)$$

for  $p \neq 1$ , and

$$S[\rho_{n,0,0}] = 2D \ln n + (2 - D) \ln 2 + \ln \pi - D \ln Z + D - 3 + S(\mathcal{Y}_{0,0}) + o(1) \quad (34)$$

for the Rényi and Shannon entropy of the ( $ns$ )-Rydberg hydrogenic states, respectively, where  $f(p, D)$  and  $S(\mathcal{Y}_{0,0})$  have the values (see Appendix A):

$$\begin{aligned} f(p, D) &= \int_{\Omega_{D-1}} |\mathcal{Y}_{0,0}(\Omega_{D-1})|^{2p} d\Omega_{D-1} \\ &= 2^{D(1-p)} \pi^{\frac{1}{2}(-Dp+D+p-1)} \left[ \frac{\Gamma(D)}{\Gamma\left(\frac{D+1}{2}\right)} \right]^{p-1} \end{aligned} \quad (35)$$

and

$$\begin{aligned} S(\mathcal{Y}_{0,0}) &= -\ln \mathcal{N}_{0,0}^2 \\ &= D \ln 2 + \frac{D-1}{2} \ln \pi + \ln \frac{\Gamma\left(\frac{D+1}{2}\right)}{\Gamma(D)}, \end{aligned} \quad (36)$$

respectively. Note that  $\lim_{p \rightarrow +1} \frac{1}{1-p} \ln f(D, p) = S(\mathcal{Y}_{0,0})$ . In the particular case  $D = 3$  (i.e., for real hydrogenic systems), one has that  $\lim_{p \rightarrow +1} \frac{1}{1-p} \ln f(3, p) = S(\mathcal{Y}_{0,0}) = \ln(4\pi)$ , as expected.

Finally, for illustrative purposes, we first numerically investigate the dependence of the Rényi entropy  $R_p[\rho_{n,0,0}]$  for some Rydberg ( $ns$ )-states on the quantum number  $n$ , the order parameter  $p$  and the nuclear charge  $Z$ . First, we study the variation of the  $p$ -th order Rényi entropy of these states in terms of  $n$ , within the interval  $n = 50 - 200$ , when  $p$  is fixed. As an example, the cases  $p = \frac{5}{4}, \frac{10}{7}, \frac{3}{4}, 3$  for the  $D$ -dimensional hydrogenic Rydberg ( $ns$ )-states with  $D = 6, 5, 4$ , and 2, respectively, are plotted in Fig. 1. We observe that the behavior of the Rényi entropy has always an increasing character for any dimensionality  $D > 2$ .

Second, in Fig. 2, we analyze the dependence of the Rényi entropy,  $R_p[\rho]$ , on the order  $p$  for the Rydberg hydrogenic state ( $n = 100, l = 1, D = 4$ ). We observe that the Rényi entropy decreases monotonically as the integer order  $p$  is increasing. This behavior indicates that the quantities with the lowest orders (particularly the cases  $p = 1$  and  $p = 2$ , which correspond to the Shannon entropy

and the disequilibrium or second-order Rényi entropy) are most significant for the quantification of the spreading of the electron distribution of the system. In fact, this behavior occurs for all the  $D$ -dimensional states; we should expect it since the Rényi entropy is defined by (1) as a continuous and non-increasing function in  $p$ .

Third, in Fig. 3, we illustrate the behavior of the Rényi entropy,  $R_p[\rho]$ , as a function of the atomic number  $Z$  of the Rydberg hydrogenic states ( $n = 100, l = 0$ ) with ( $p = 3, D = 2$ ) and ( $p = \frac{3}{4}, D = 4$ ), where  $Z$  goes from 1 (hydrogen) to 103 (lawrencium). We observe that the Rényi entropy decreases monotonically as  $Z$  increases, which points out the fact that the probability distribution of the system tends to separate out from equiprobability more and more as the number of electrons in the nucleus of the atom increases; so, quantifying the greater complexity of the system as the atomic number grows.

Finally, we investigate the behavior of the Rényi entropy,  $R_p[\rho]$ , of the Rydberg hydrogenic state as a function of the dimensionality  $D$ . We show it in Fig. 4 for the Rydberg state ( $n = 100, l = 0$ ) with  $p = \frac{1}{2}$  and 4 of the hydrogen atom with various integer values of the dimensionality  $D \in [50, 200]$ . We observe that in both cases the Rényi entropy has a monotonically increasing behavior as  $D$  grows, which indicates that the larger the dimension, more classically the system behaves (or in other words, the closer is the system to its classical counterpart).

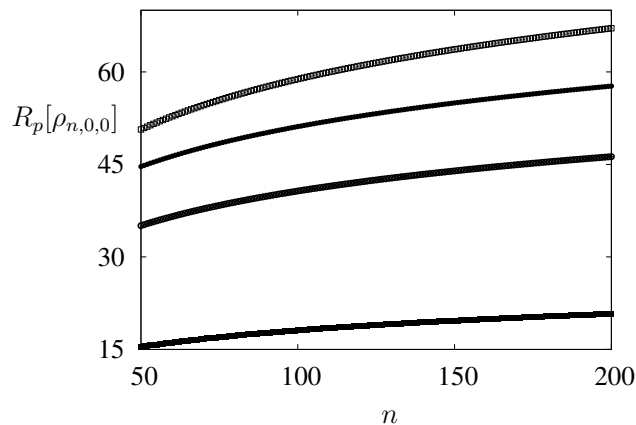


FIG. 1: Variation of the Rényi entropy,  $R_p[\rho]$ , with respect to  $n$  for the Rydberg hydrogenic ( $ns$ )-states with ( $p = \frac{5}{4}, D = 6$ )( $\square$ ), ( $p = \frac{10}{7}, D = 5$ )( $\bullet$ ), ( $p = \frac{3}{4}, D = 4$ )( $\circ$ ) and ( $p = 3, D = 2$ )( $\blacksquare$ ).

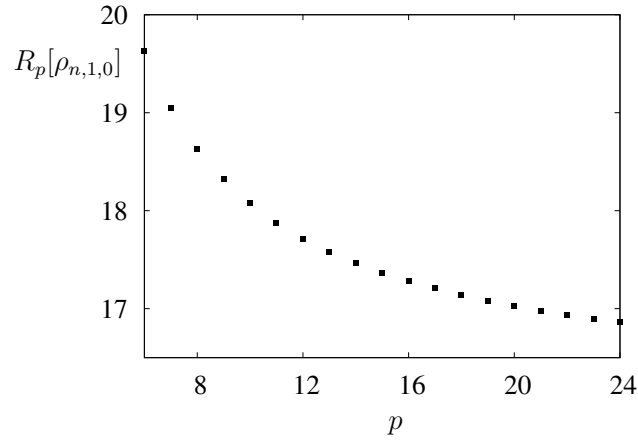


FIG. 2: Variation of the Rényi entropy  $R_p[\rho_{n,1,0}]$ , respectively, with respect to  $p$  for the Rydberg state ( $n = 100, l = 1$ ) of the hydrogen atom ( $Z = 1$ ) with  $D = 4$ .

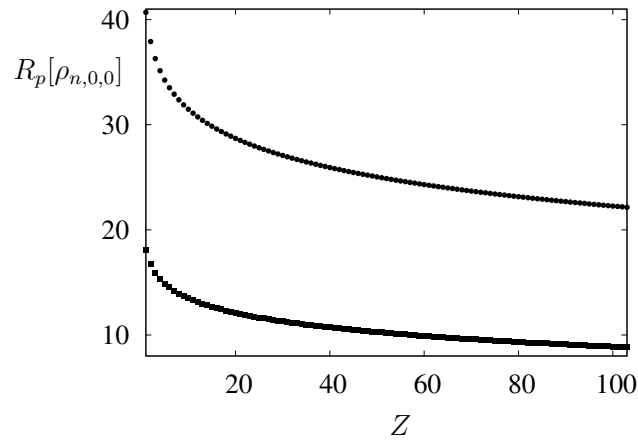


FIG. 3: Variation of the Rényi entropy,  $R_p[\rho]$ , with respect to the nuclear charge  $Z$  for the Rydberg hydrogenic state ( $n = 100, l = 0$ ) of the  $D$ -dimensional hydrogen atom with  $D = 2$  (■) and  $D = 4$  (●).

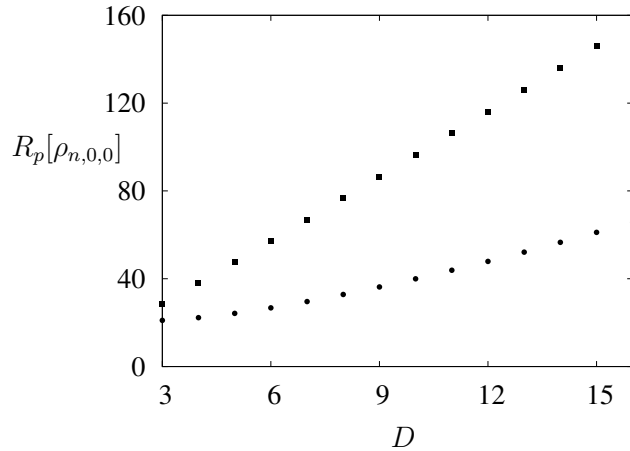


FIG. 4: Variation of the Rényi entropy,  $R_p[\rho]$ , with respect to the dimensionality  $D$  for the Rydberg hydrogenic state ( $n = 100, l = 0$ ) of the  $D$ -dimensional hydrogen atom with  $p = \frac{1}{2}$  (■) and  $p = 4$  (●).

## V. CONCLUSIONS

In this work we determine the three main entropic measures (Rényi, Shannon, Tsallis) of the quantum probability density of all stationary  $D$ -dimensional Rydberg ( $n \gg 1$ ) hydrogenic states in terms of the basic parameters which characterize them; namely, the dimensionality  $D$ , the hyperquantum numbers ( $n, l, \{\mu\}$ ) and the nuclear charge  $Z$  of the system. In fact, the Shannon and Tsallis entropies can be obtained from the Rényi one. The Rényi entropy has been calculated by first decomposing it into two parts of radial and angular types, and realizing that the angular part does not depend on  $n$ , so that the true problem to be solved is the calculation of the radial Rényi entropy in the limit of large  $n$ . The radial Rényi entropy has been shown to be expressed in terms of the  $\mathfrak{L}_p$ -norms of the Laguerre polynomials which control the Rydberg states we are interested in. Then, the remaining asymptotics of these Laguerre norms is determined by means of a recent technique of approximation theory. Finally, we numerically apply this theoretical methodology to some particular Rydberg hydrogenic states of  $s$  and  $p$  types. We find that the Rényi entropy monotonically decreases (increases) when the nuclear charge (the dimensionality) is decreasing (increasing) for some  $s$  and  $p$  states.

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### Appendix A: Calculation of $f(p, D)$ and $S(\mathcal{Y}_{0,0})$

Let us first calculate the factor  $f(p, D)$  which appears in Eq. (33):

$$\begin{aligned}
 f(p, D) &= \int_{\Omega_{D-1}} |\mathcal{Y}_{0,0}(\Omega_{D-1})|^{2p} d\Omega_{D-1} \\
 &= \int_{\Omega_{D-1}} (\mathcal{N}_{0,0}^2)^p d\Omega_{D-1} \\
 &= (\mathcal{N}_{0,0}^2)^p 2\pi \prod_{j=1}^{D-2} \frac{\sqrt{\pi} \Gamma\left(\frac{D-j}{2}\right)}{\Gamma\left(\frac{1}{2}(D-j+1)\right)} \\
 &= (2\pi)^{1-p} \left[ \prod_{j=1}^{D-2} \frac{(D-j-1)\Gamma\left(\frac{1}{2}(D-j-1)\right)^2}{\pi 2^{-D+j+3}\Gamma(D-j-1)} \right]^p \prod_{j=1}^{D-2} \frac{\sqrt{\pi} \Gamma\left(\frac{D-j}{2}\right)}{\Gamma\left(\frac{1}{2}(D-j+1)\right)}, \\
 &= 2^{1-p} \pi^{\frac{D}{2}(1-p)} \left[ \prod_{j=1}^{D-2} \frac{\Gamma\left(\frac{1}{2}(D-j+1)\right)}{\Gamma\left(\frac{D-j}{2}\right)} \right]^p \prod_{j=1}^{D-2} \frac{\Gamma\left(\frac{D-j}{2}\right)}{\Gamma\left(\frac{1}{2}(D-j+1)\right)} \\
 &= 2^{1-p} \pi^{\frac{D}{2}(1-p)} \left[ \Gamma\left(\frac{D}{2}\right) \right]^{p-1}
 \end{aligned} \tag{A1}$$

Let us now compute the factor  $S(\mathcal{Y}_{0,0})$  which appears in Eq. (34):

$$\begin{aligned}
 S(\mathcal{Y}_{0,0}) &= -\ln \mathcal{N}_{0,0}^2 \\
 &= -\ln \left[ \frac{1}{2\pi} \prod_{j=1}^{D-2} \frac{(D-j-1)\Gamma(\frac{1}{2}(D-j-1))^2}{\pi 2^{-D+j+3}\Gamma(D-j-1)} \right], \\
 &= \ln 2\pi - \ln \prod_{j=1}^{D-2} \frac{\Gamma(\frac{1}{2}(D-j+1))}{\sqrt{\pi}\Gamma(\frac{D-j}{2})} \\
 &= \ln 2\pi - \left(1 - \frac{D}{2}\right) \ln \pi - \ln \prod_{j=1}^{D-2} \frac{\Gamma(\frac{1}{2}(D-j+1))}{\Gamma(\frac{D-j}{2})} \\
 &= \ln 2\pi - \left(1 - \frac{D}{2}\right) \ln \pi - \ln \Gamma\left(\frac{D}{2}\right) \\
 &= \ln 2 + \frac{D}{2} \ln \pi - \ln \frac{2^{1-D}\pi^{1/2}(D-1)!}{(\frac{D-1}{2})!} \\
 &= D \ln 2 + \frac{D-1}{2} \ln \pi + \ln \frac{\Gamma(\frac{D+1}{2})}{\Gamma(D)}.
 \end{aligned} \tag{A2}$$

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## 2.2 High-dimensional states

Witten, Herschbach and other authors [12, 13, 15–19, 147, 153, 154] realize the relevance of the investigation of the properties of the pseudoclassical or high-dimensional states of numerous systems from atoms, molecules and fluids up until quarks and gluons. Basically, this is because physics in the large- $D$  limit becomes much simpler. Indeed, in this limit the electrons of a many-electron system assume fixed positions relative to the nuclei and each other, in the  $D$ -scaled space. Moreover, the large- $D$  electronic geometry and energy correspond to the minimum of an exactly known effective potential and can be determined from classical electrostatics for any atom or molecule, what remembers the prequantum models of Lewis and Langmuir.

The spreading properties of the electronic distribution of the  $D$ -dimensional hydrogenic atom have been analyzed by means of its moments around the origin (radial expectation values) in both position and momentum spaces [41, 48, 155]. These quantities are formally given in terms of  $D$ , the hyperquantum numbers of the hydrogenic states and the nuclear charge  $Z$  through a generalized hypergeometric function  ${}_{p+1}F_p(1)$ , which cannot be easily calculated unless the hyperquantum numbers and/or the dimension  $D$  are sufficiently small. However, for the high-dimensional (pseudo-classical) states the position and momentum moments around the origin of the  $D$ -dimensional hydrogenic atom have been determined [41, 48] in a simple and compact form by means of powerful asymptotical tools of the modern approximation theory related to the varying Laguerre and Gegenbauer polynomials which control the corresponding position and momentum wavefunctions.

In this section we extend the previous work by determining in an analytical way the entropic uncertainty measures, precisely the Rényi entropies, of the high-dimensional hydrogenic system in position and momentum spaces and their associated uncertainty relation in terms of the state's hyperquantum numbers and the nuclear charge  $Z$  of the system. This has been carried out through the asymptotics ( $\alpha \rightarrow \infty$ ) of the Laguerre  $\mathcal{L}_k^{(\alpha)}(x)$  and Gegenbauer  $\mathcal{C}_k^{(\alpha)}(x)$  polynomials given by Theorems 1.3 and 1.4 of Temme et al discussed in subsection 1.2.2.

Specifically, the following results have been achieved:

- The Rényi entropies with a natural parameter have been explicitly determined for the pseudoclassical (high-D) states of the  $D$ -dimensional hydrogenic system in both position and momentum spaces.
- The dependence of the Rényi entropies for these high-dimensional states on the main hyperquantum number  $n$ , is obtained and discussed.
- Especially simple expressions of these quantities for some concrete classes of hydrogenic states ( $ns$  and circular states), which include the ground state, are given.

- Saturation of the known position-momentum Rényi-entropy-based uncertainty relations of Bilaynicki-Birula-Zozor-Vignat [91–93] is reached. To this respect we should keep in mind that we are assuming that the dimensionality is very large and the hyperquantum numbers are small. The exceptional case when both dimensionality and hyperquantum numbers are simultaneously large has not yet been explored; in particular, we cannot assure saturation.

These results have been published [63] in the article with coordinates: **Puertas-Centeno D.**, Temme N. M., Toranzo I. V. and Dehesa J. S. *Entropic uncertainty measures for large dimensional hydrogenic systems*. *Journal of Mathematical Physics*, 58:103302, 2017, which is attached below.

# Entropic uncertainty measures for large dimensional hydrogenic systems

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The entropic moments of the probability density of a quantum system in position and momentum spaces describe not only some fundamental and/or experimentally accessible quantities of the system, but also the entropic uncertainty measures of Rényi type which allow one to find the most relevant mathematical formalizations of the position-momentum Heisenberg's uncertainty principle, the entropic uncertainty relations. It is known that the solution of difficult three-dimensional problems can be very well approximated by a series development in  $1/D$  in similar systems with a non-standard dimensionality  $D$ ; moreover, several physical quantities of numerous atomic and molecular systems have been numerically shown to have values in the large- $D$  limit comparable to the corresponding ones provided by the three-dimensional numerical self-consistent field methods. The  $D$ -dimensional hydrogenic atom is the main prototype of the physics of multidimensional many-electron systems. In this work we rigorously determine the leading term of the Rényi entropies of the  $D$ -dimensional hydrogenic atom at the limit of large  $D$ . As a byproduct, we show that our results saturate the known position-momentum Rényi-entropy-based uncertainty relations.

Keywords: Entropic uncertainty measures,  $D$ -dimensional hydrogenic systems,  $D$ -dimensional quantum physics, radial and momentum expectation values, hydrogenic states at large dimensions

## I. INTRODUCTION

In an excellent tutorial article about quarks, gluons and *impossible problems* of quantum chromodynamics, Edward Witten [1] illustrated the utility of the large-dimension  $D$  limit with a rough calculation for helium. This prompted Dudley R. Herschbach et al [3, 4] and other authors (see the review [2]) to develop a new strategy, the dimensional scaling method, to solve first the quantum problems with one degree of freedom [2] and later the much more difficult Coulomb problems involving two or more non-separable, strongly-coupled degrees of freedom which usually take place in physics of atoms and molecules [3, 4]. With this method a finite many-body problem is typically solved in the large- $D$  limit, most often in an analytical way, and then perturbation theory in  $1/D$  is used to obtain an approximate result for the standard dimension ( $D = 3$ ).

Physics in the large- $D$  limit becomes much simpler. Indeed, in this limit the electrons of a many-electron system assume fixed positions relative to the nuclei and each other, in the  $D$ -scaled space. Moreover, the large- $D$  electronic geometry and energy correspond to the minimum of an exactly known effective potential and can be determined from classical electrostatics for any atom or molecule, what remembers the prequantum models of Lewis and Langmuir [5, 6]. The ( $D \rightarrow \infty$ )-limit is called *pseudoclassical*, tantamount to  $\hbar \rightarrow 0$  and/or  $m_e \rightarrow \infty$  in the kinetic energy. This limit is not the same as the conventional classical limit obtained by  $\hbar \rightarrow 0$  for a fixed dimension [7, 8]. Although at first sight the electrons at rest in fixed locations might seem violate the uncertainty principle, this is not true because that occurs only in the  $D$ -scaled space (see e.g., [6]). For  $D$  finite but very large, the electrons are confined to harmonic oscillations about the fixed positions attained in the ( $D \rightarrow \infty$ )-limit. Moreover, the large- $D$  limit of numerous physical properties of almost all atoms with up to 100 electrons and many diatomic molecules have been numerically evaluated, obtaining values comparable to or better than single-zeta Hartree-Fock calculations [3, 4, 9].

The main prototype of the  $D$ -dimensional Coulomb many-body systems, the  $D$ -dimensional hydrogen atom (i.e., a negatively-charged particle moving in a space of  $D$  dimensions around a positively charged core which electromagnetically binds it in its orbit), has been investigated in detail starting from its wave functions which are analytically known [10–12] in the two conjugated position and momentum spaces for any dimension. This system includes a wide variety of physical objects, such as e.g. hydrogenic atoms and ions, some exotic atoms and antimatter atoms, excitons in semiconductors and qubits.

The spreading properties of the electronic distribution of the  $D$ -dimensional hydrogenic atom have been analyzed by means of its moments around the origin (radial expectation values) in both position [13–18] and momentum [19, 20] spaces. However, these quantities are formally given in terms of  $D$ , the hyperquantum numbers of the hydrogenic states and the nuclear charge  $Z$  through a generalized hypergeometric function  ${}_{p+1}F_p(1)$ , which cannot be easily calculated unless the hyperquantum numbers and/or the dimension  $D$  are sufficiently small. Recently the position and momentum moments around the origin of the  $D$ -dimensional hydrogenic atom have been determined in a simple and compact form for the highly and very-highly excited (i.e., Rydberg) states [12, 21] as well as for any excited state at large  $D$  [22].

The determination of the entropic measures of the  $D$ -dimensional hydrogenic atom, which describe most appropriately the electronic uncertainty of the system, is far more difficult except for the lowest-lying energy states despite some efforts [12]. This is because these quantities are described by means of some power or logarithmic functionals of the electron density, which cannot be calculated in an analytical way nor numerically computed; the latter is basically because a naive numerical evaluation using quadratures is not convenient due to the increasing number of integrable singularities when the principal hyperquantum number  $n$  is increasing, which spoils any attempt to achieve reasonable accuracy even for rather small  $n$  [23]. Recently, the main entropic properties of the  $D$ -dimensional Rydberg hydrogenic states (namely, the Rényi, Shannon and Tsallis entropies) have been explicitly calculated in a compact form [24, 25] by use of modern techniques of approximation theory based on the strong asymptotics ( $n \rightarrow \infty$ ) of the Laguerre  $\mathcal{L}_n^{(\alpha)}(x)$  and Gegenbauer  $\mathcal{C}_n^{(\alpha)}(x)$  polynomials ( $x$ ) which control the state's wave functions in position and momentum spaces, respectively [26].

In this work we first determine the Rényi entropy and then we conjecture the Shannon entropy in both position and momentum spaces for the large-dimensional hydrogenic states in terms of the dimensionality  $D$ , the nuclear charge  $Z$  and the principal and orbital hyperquantum numbers of the states. The Rényi entropies  $R_q[\rho]$ ,  $q > 0$  are defined [27, 28] as

$$R_q[\rho] = \frac{1}{1-q} \log \int_{\mathbb{R}^D} [\rho(\vec{r})]^q d\vec{r}, \quad q \neq 1. \quad (1)$$

Note that the Shannon entropy  $S[\rho] = - \int \rho(\vec{r}) \log \rho(\vec{r}) d\vec{r} = \lim_{q \rightarrow 1} R_q[\rho]$ ; see e.g. [29]. These quantities completely characterize the density  $\rho(\vec{r})$  [30] under certain conditions. In fact, we can cal-



culate from (1) other relevant entropic quantities such as e.g. the disequilibrium  $\langle \rho \rangle = \exp(-R_2[\rho])$ , and the Tsallis entropies  $T_q[\rho] = \frac{1}{q-1} (1 - \int_{\mathbb{R}^D} [\rho(\vec{r})]^q d\vec{r})$ ,  $q > 0$  [31] as

$$T_q[\rho] = \frac{1}{1-q} [e^{(1-q)R_q[\rho]} - 1]. \quad (2)$$

which holds for  $q \neq 1$ . Here again, the Shannon entropy  $S[\rho] = \lim_{q \rightarrow 1} T_q[\rho]$ . The properties of the Rényi entropies and their applications have been widely considered; see e.g. [29, 32, 33] and the reviews [34–36]. The use of Rényi and Shannon entropies as measures of uncertainty allow a wider quantitative range of applicability than the moments around the origin and the standard or root-square-mean deviation do. This permits, for example, a quantitative discussion of quantum uncertainty relations further beyond the conventional Heisenberg-like uncertainty relations [22, 34, 35, 37].

The structure of this work is the following. In section II the wave functions of the  $D$ -dimensional hydrogenic states in both position and momentum spaces are briefly described, and the corresponding probability densities are given. In section III we determine the physical Rényi entropies of the  $D$ -dimensional hydrogenic atom at large  $D$  by use of some recent theorems relative to the asymptotics ( $\alpha \rightarrow \infty$ ) of the underlying Rényi-like integral functionals of Laguerre polynomials  $\mathcal{L}_k^{(\alpha)}(x)$  and Gegenbauer polynomials  $\mathcal{C}_k^{(\alpha)}(x)$  which control the hydrogenic wavefunctions as described in the previous section. The dominant term of the joint position-momentum uncertainty sum for the general states of the large dimensional hydrogenic systems is also given and, what is most interesting, shown to saturate the known position-momentum Rényi-entropy-based uncertainty relations [38–40]. Finally, some conclusions, open problems and three appendices are given.

## II. THE $D$ -DIMENSIONAL HYDROGENIC PROBLEM: BASICS

In this section we briefly summarize the physical solutions of the Schrödinger equation of the  $D$ -dimensional hydrogenic system in both position and momentum spaces. Then we give the associated position and momentum  $D$ -dimensional probability densities of the system.

The time-independent Schrödinger equation of a  $D$ -dimensional ( $D > 1$ ) hydrogenic system (i.e., an electron moving under the action of the  $D$ -dimensional Coulomb potential  $V(\vec{r}) = -\frac{Z}{r}$ ) is given by

$$\left( -\frac{1}{2} \vec{\nabla}_D^2 - \frac{Z}{r} \right) \Psi(\vec{r}) = E \Psi(\vec{r}), \quad (3)$$

where  $\vec{\nabla}_D$  denotes the  $D$ -dimensional gradient operator,  $Z$  is the nuclear charge, and the electronic position vector  $\vec{r} = (x_1, \dots, x_D)$  in hyperspherical units is given as  $(r, \theta_1, \theta_2, \dots, \theta_{D-1}) \equiv (r, \Omega_{D-1})$ ,  $\Omega_{D-1} \in S^{D-1}$ , where  $r \equiv |\vec{r}| = \sqrt{\sum_{i=1}^D x_i^2} \in [0, +\infty)$  and  $x_i = r \left( \prod_{k=1}^{i-1} \sin \theta_k \right) \cos \theta_i$  for  $1 \leq i \leq D$  and with  $\theta_i \in [0, \pi)$ ,  $i < D-1$ ,  $\theta_{D-1} \equiv \phi \in [0, 2\pi)$ . It is assumed that the nucleus is located at the origin and, by convention,  $\theta_D = 0$  and the empty product is the unity. Atomic units are used throughout the paper.

It is known [10–12] that the energies belonging to the discrete spectrum are given by

$$E = -\frac{Z^2}{2\eta^2}, \quad \eta = n + \frac{D-3}{2}; \quad n = 1, 2, 3, \dots, \quad (4)$$

and the associated eigenfunction can be expressed as

$$\Psi_{n,l,\{\mu\}}(\vec{r}) = \mathcal{R}_{n,l}(r) \mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}), \quad (5)$$

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

$$\begin{aligned} \mathcal{R}_{n,l}(r) &= \mathfrak{N}_{n,l} \left( \frac{r}{\lambda} \right)^l e^{-\frac{r}{2\lambda}} \mathcal{L}_{n-l-1}^{(2l+D-2)} \left( \frac{r}{\lambda} \right) \\ &= \mathfrak{N}_{n,l} \left[ \frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}} \right]^{1/2} \mathcal{L}_{\eta-L-1}^{(2L+1)}(\tilde{r}) \\ &= \left( \frac{\lambda^{-D}}{2\eta} \right)^{1/2} \left[ \frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}} \right]^{1/2} \widehat{\mathcal{L}}_{\eta-L-1}^{(2L+1)}(\tilde{r}), \end{aligned} \quad (6)$$

where the “grand orbital angular momentum quantum number”  $L$  and the dimensionless parameter  $\tilde{r}$  are

$$L = l + \frac{D-3}{2}, \quad l = 0, 1, 2, \dots \quad (7)$$

$$\tilde{r} = \frac{r}{\lambda}, \quad \lambda = \frac{\eta}{2Z}, \quad (8)$$

and  $\omega_\alpha(x) = x^\alpha e^{-x}$ ,  $\alpha = 2L+1 = 2l+D-2$ , is the weight function of the Laguerre polynomials  $\mathcal{L}_k^{(\alpha)}(x)$ ,  $x \in [0, \infty)$ . Note that  $\alpha \geq 0$  for  $D \geq 2$ . The symbols  $\mathcal{L}_k^{(\alpha')}(x)$  and  $\widehat{\mathcal{L}}_k^{(\alpha')}(x)$  denote the orthogonal and orthonormal Laguerre polynomials, so that

$$\widehat{\mathcal{L}}_k^{(\alpha')}(x) = \left( \frac{k!}{\Gamma(k + \alpha' + 1)} \right)^{1/2} \mathcal{L}_k^{(\alpha')}(x), \quad (9)$$

for any parameter  $\alpha' > -1$ , and finally

$$\mathfrak{N}_{n,l} \equiv \lambda^{-\frac{D}{2}} \left\{ \frac{(\eta-L-1)!}{2\eta(\eta+L)!} \right\}^{\frac{1}{2}} = \left\{ \left( \frac{2Z}{n + \frac{D-3}{2}} \right)^D \frac{(n-l-1)!}{2 \left( n + \frac{D-3}{2} \right) (n+l+D-3)!} \right\}^{\frac{1}{2}} \quad (10)$$

represents the normalization constant which ensures that  $\int |\Psi_{n,l,\{\mu\}}(\vec{r})|^2 d\vec{r} = 1$ . Note that the  $D$ -dimensional volume element is  $d\vec{r} \equiv d^D r = r^{D-1} dr d\Omega_{D-1}$  and

$$d\Omega_{D-1} = \left( \prod_{j=1}^{D-2} (\sin \theta_j)^{2\alpha_j} d\theta_j \right) d\theta_{D-1},$$

where  $2\alpha_j = D - j - 1$ . The angular eigenfunctions are the hyperspherical harmonics,  $\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})$ , defined [10, 12, 42] as

$$\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) = \mathcal{N}_{l,\{\mu\}} e^{im\phi} \times \prod_{j=1}^{D-2} C_{\mu_j - \mu_{j+1}}^{(\alpha_j + \mu_{j+1})}(\cos \theta_j) (\sin \theta_j)^{\mu_{j+1}} \quad (11)$$

with the squared normalization constant given as

$$\begin{aligned} \mathcal{N}_{l,\{\mu\}}^2 &= \frac{1}{2\pi} \prod_{j=1}^{D-2} \frac{(\alpha_j + \mu_j)(\mu_j - \mu_{j+1})! [\Gamma(\alpha_j + \mu_{j+1})]^2}{\pi 2^{1-2\alpha_j-2\mu_{j+1}} \Gamma(2\alpha_j + \mu_j + \mu_{j+1})}, \\ &= \frac{1}{2\pi} \prod_{j=1}^{D-2} A_{\mu_j, \mu_{j+1}}^{(j)}, \end{aligned} \quad (12)$$

where the symbol  $C_k^{(\alpha')}(t)$  denotes the Gegenbauer polynomial [41] of degree  $k$  and parameter  $\alpha'$ . Then, the quantum probability density of a  $D$ -dimensional hydrogenic stationary state  $(n, l, \{\mu\})$  is given in position space by the the squared modulus of the position eigenfunction given by (5) as

$$\rho_{n,l,\{\mu\}}(\vec{r}) = \rho_{n,l}(\tilde{r}) |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2, \quad (13)$$

where the radial part of the density is the univariate radial density function

$$\rho_{n,l}(\tilde{r}) = [\mathcal{R}_{n,l}(r)]^2 = \frac{\lambda^{-D}}{2\eta} \frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}} [\widehat{\mathcal{L}}_{\eta-L-1}^{(2L+1)}(\tilde{r})]^2. \quad (14)$$

On the other hand, the Fourier transform of the position eigenfunction  $\Psi_{n,l,\{\mu\}}(\vec{r})$  given by (5) provides the eigenfunction of the system in the conjugated momentum space as

$$\tilde{\Psi}_{n,l,\{\mu\}}(\vec{p}) = \mathcal{M}_{n,l}(p) \mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}), \quad (15)$$

where the radial part is

$$\mathcal{M}_{n,l}(p) = K_{n,l} \frac{(\eta \tilde{p})^l}{(1 + \eta^2 \tilde{p}^2)^{L+2}} C_{\eta-L-1}^{(L+1)} \left( \frac{1 - \eta^2 \tilde{p}^2}{1 + \eta^2 \tilde{p}^2} \right) \quad (16)$$

with  $\tilde{p} = \frac{p}{Z}$  and the normalization constant

$$K_{n,l} = Z^{-\frac{D}{2}} 2^{2L+3} \left[ \frac{(\eta - L - 1)!}{2\pi(\eta + L)!} \right]^{\frac{1}{2}} \Gamma(L + 1) \eta^{\frac{D+1}{2}}. \quad (17)$$

Then, the expression

$$\begin{aligned} \gamma_{n,l,\{\mu\}}(\vec{p}) &= |\tilde{\Psi}_{n,l,\{\mu\}}(\vec{p})|^2 = \mathcal{M}_{n,l}^2(p) |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2 \\ &= K_{n,l}^2 \frac{(\eta\tilde{p})^{2l}}{(1 + \eta^2\tilde{p}^2)^{2L+4}} \left[ \mathcal{C}_{\eta^{-L-1}}^{(L+1)} \left( \frac{1 - \eta^2\tilde{p}^2}{1 + \eta^2\tilde{p}^2} \right) \right]^2 |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2 \end{aligned} \quad (18)$$

gives the momentum probability density of the  $D$ -dimensional hydrogenic stationary state with the hyperquantum numbers  $(n, l, \{\mu\})$ .

### III. RÉNYI ENTROPIES OF LARGE DIMENSIONAL HYDROGENIC STATES

In this section we obtain the Rényi entropies of a generic  $D$ -dimensional hydrogenic state  $(n, l, \{\mu\})$  in the large- $D$  limit in both position and momentum spaces. We start with the expressions (13) and (18) of the position and momentum probability densities of the system, respectively.

To calculate the position Rényi entropy we decompose it into two radial and angular parts. The radial part is first expressed in terms of a Rényi-like integral functional of Laguerre polynomials  $\mathcal{L}_{n-l-1}^{(\alpha)}(x)$  with  $\alpha = D + 2l - 2$ , and then this functional is determined in the large- $D$  limit by means of Theorem 1 (see Appendix A). The angular part is given by a Rényi-like integral functional of hyperspherical harmonics, which can be expressed in terms of Rényi-like functionals of Gegenbauer polynomials  $\mathcal{C}_{n-l-1}^{(\alpha')}$  with  $\alpha' = D/2 + l - 1/2$ ; later on, we evaluate these Gegenbauer functionals at large  $D$  by means of Theorem 2 (see Appendix B), with emphasis in the circular and ( $ns$ ) states which are characterized by the hyperquantum numbers  $(n, l = n - 1, \{\mu\} = \{n - 1\})$  and  $(n, l = 0, \{\mu\} = \{0\})$ , respectively.

Operating similarly in momentum space we can determine the momentum Rényi entropy of the system. In this space both the radial and angular parts of the momentum wave functions of the hydrogenic states are controlled by Gegenbauer polynomials as follows from the previous section. Consequently, the two radial and angular contributions to the momentum Rényi entropy are expressed in terms of Rényi-like functionals of Gegenbauer polynomials.

### A. Rényi entropy in position space

Let us obtain the position Rényi entropy of the probability density  $\rho_{n,l,\{\mu\}}(\vec{r})$  given by (13), which according to (1) is defined as

$$R_q[\rho_{n,l,\{\mu\}}] = \frac{1}{1-q} \log W_q[\rho_{n,l,\{\mu\}}]; \quad 0 < q < \infty, \quad q \neq 1, \quad (19)$$

where the symbol  $W_q[\rho_{n,l,\{\mu\}}]$  denotes the entropic moments of the density

$$\begin{aligned} W_q[\rho_{n,l,\{\mu\}}] &= \int_{\mathbb{R}^D} [\rho_{n,l,\{\mu\}}(\vec{r})]^q d\vec{r} \\ &= \int_0^\infty [\rho_{n,l}(\tilde{r})]^q r^{D-1} dr \times \Lambda_{l,\{\mu\}}(\Omega_{D-1}), \end{aligned} \quad (20)$$

with the angular part given by

$$\Lambda_{l,\{\mu\}}(\Omega_{D-1}) = \int_{S^{D-1}} |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^{2q} d\Omega_{D-1}. \quad (21)$$

Then, from Eqs. (20) and (19) we can obtain the Rényi entropies of the  $D$ -dimensional hydrogenic state  $(n, l, \{\mu\})$  as follows

$$R_q[\rho_{n,l,\{\mu\}}] = R_q[\rho_{n,l}] + R_q[\mathcal{Y}_{l,\{\mu\}}], \quad (22)$$

where  $R_q[\rho_{n,l}]$  denotes the radial part

$$R_q[\rho_{n,l}] = \frac{1}{1-q} \log \int_0^\infty [\rho_{n,l}(\tilde{r})]^q r^{D-1} dr, \quad (23)$$

and  $R_q[\mathcal{Y}_{l,\{\mu\}}]$  denotes the angular part

$$R_q[\mathcal{Y}_{l,\{\mu\}}] = \frac{1}{1-q} \log \Lambda_{l,\{\mu\}}(\Omega_{D-1}). \quad (24)$$

Here our aim is to determine the large- $D$  behavior of the Rényi entropy  $R_q[\rho_{n,l,\{\mu\}}]$  when all the hyperquantum numbers are fixed. According to (22) this issue requires the knowledge at  $D \gg 1$  of the radial and angular Rényi entropies, i.e.  $R_q[\rho_{n,l}]$  and  $R_q[\mathcal{Y}_{l,\{\mu\}}]$  respectively, whose determination is done in the following.

#### 1. Radial position Rényi entropy

According to Eq. (23), the radial Rényi entropy can be expressed as

$$R_q[\rho_{n,l}] = \frac{1}{1-q} \log \left[ \frac{\eta^{D(1-q)-q}}{2^{D(1-q)+q} \mathcal{Z}^{D(1-q)}} N_{n,l}(D, q) \right], \quad (25)$$

where  $N_{n,l}(D, q)$  denotes the following  $\mathfrak{L}_q$ -norm of the Laguerre polynomials

$$N_{n,l}(D, q) = \int_0^\infty \left( \left[ \widehat{\mathcal{L}}_{n-l-1}^{(\alpha)}(x) \right]^2 w_\alpha(x) \right)^q x^\beta dx, \quad (26)$$

with  $\tilde{r} \equiv x$  and

$$\alpha = D + 2l - 2, \quad l = 0, 1, 2, \dots, n - 1, \quad q > 0 \quad \text{and} \quad \beta = (2 - D)q + D - 1. \quad (27)$$

We note that (27) guarantees the convergence of integral (26); i.e., the condition  $\beta + q\alpha = 2lq + D - 1 > -1$  is always satisfied for physically meaningful values of the parameters. Moreover, the norm  $N_{n,l}(D, q)$  can be rewritten as

$$\begin{aligned} N_{n,l}(D, q) &= \int_0^\infty \left( \left[ \widehat{\mathcal{L}}_{n-l-1}^{(D+2l-2)}(x) \right]^2 w_{D+2l-2}(x) \right)^q x^{2q-1+(1-q)D} dx \\ &= \left[ \frac{\Gamma(n-l)}{\Gamma(n+l+D-2)} \right]^q \int_0^\infty x^{D+2lq-1} e^{-qx} \left[ \mathcal{L}_{n-l-1}^{(D+2l-2)}(x) \right]^{2q} dx. \end{aligned} \quad (28)$$

Then, the determination of the large- $D$  behavior of the radial Rényi entropy  $R_q[\rho_{n,l}]$  requires the calculation of the asymptotics of the Laguerre functional  $N_{n,l}(D, q)$  defined by (26); that is, the evaluation of the Rényi-like integral functional given by (28) when  $D \gg 1$ . We do it by applying Theorem 1 (see Appendix A) to the functional  $N_{n,l}(D, q)$  given by (28) with  $(n, l)$  fixed, obtaining for every non-negative  $q \neq 1$  that

$$\begin{aligned} N_{n,l}(D, q) &\sim \left[ \frac{\Gamma(n-l)}{\Gamma(n+l+D-2)} \right]^q \frac{\sqrt{2\pi}}{[\Gamma(n-l)]^{2q}} |q-1|^{2(n-l-1)q} \\ &\quad \times e^{-D-2l+2} (D+2(l-1))^{D+2q(n-1)-\frac{1}{2}} q^{-D-2q(n-1)} \\ &= \frac{\sqrt{2\pi} |q-1|^{2(n-l-1)q}}{\Gamma(n-l)^q} e^{-D-2l+2} \frac{(D+2l-2)^{D+2q(n-1)-\frac{1}{2}} q^{-D-2q(n-1)}}{\Gamma(D+n+l-2)^q} \\ &\sim \frac{(2\pi)^{\frac{1-q}{2}} |q-1|^{2(n-l-1)q}}{\Gamma(n-l)^q} q^{-2q(n-1)} \left( \frac{D}{e} \right)^{D(1-q)} q^{-D} D^{q(n-l+\frac{1}{2})-\frac{1}{2}} \end{aligned} \quad (29)$$

where we have used the Stirling's formula [41] for the gamma function  $\Gamma(x) = e^{-x} x^{x-\frac{1}{2}} (2\pi)^{\frac{1}{2}} [1 + \mathcal{O}(x^{-1})]$ .

Then, Eqs. (25)-(29) allow us to find the following large- $D$  behavior for the radial Rényi entropy:

$$\begin{aligned} R_q[\rho_{n,l}] &\sim \frac{1}{1-q} \log \left\{ \frac{(2\pi)^{\frac{1-q}{2}} |q-1|^{2(n-l-1)q}}{\Gamma(n-l)^q} q^{-2q(n-1)} \frac{D^{D(1-q)-q} e^{(2n-3)(1-q)}}{4^{D(1-q)} Z^{D(1-q)}} \left( \frac{D}{e} \right)^{D(1-q)} q^{-D} D^{q(n-l+\frac{1}{2})-\frac{1}{2}} \right\} \\ &= \frac{1}{1-q} \log \left\{ \frac{(2\pi)^{\frac{1-q}{2}} |q-1|^{2(n-l-1)q}}{\Gamma(n-l)^q} \frac{e^{(2n-3)(1-q)}}{q^{2q(n-1)}} \left( \frac{D^2}{4Ze} \right)^{D(1-q)} q^{-D} D^{q(n-l-\frac{1}{2})-\frac{1}{2}} \right\} \end{aligned} \quad (30)$$

which can be rewritten as

$$R_q[\rho_{n,l}] \sim 2D \log [D] + D \log \left[ \frac{q^{\frac{1}{q-1}}}{4Ze} \right] + \frac{q(n-l-\frac{1}{2})-\frac{1}{2}}{1-q} \log D + \frac{1}{1-q} \log \mathcal{F}(n,l,q), \quad (31)$$

where  $\mathcal{F}(n,l,q) = \frac{(2\pi)^{\frac{1-q}{2}} |q-1|^{2(n-l-1)q} e^{(2n-3)(1-q)}}{\Gamma(n-l)^q q^{2q(n-1)}}$ . Further terms in this asymptotic expansion can be obtained by means of Theorem 1 (see Appendix A).

Note that, since  $q^{\frac{1}{q-1}} \rightarrow e$  when  $q \rightarrow 1$ , we have the following conjecture for the value of the Shannon entropy

$$S[\rho_{n,l}] \sim 2D \log [D] - D \log [4Z], \quad (32)$$

which can be numerically shown to be correct. However a more rigorous expression for this quantity remains to be proved.

Then, according to Eq. (22), to fix the total Rényi entropy  $R_q[\rho_{n,l,\{\mu\}}]$  at large  $D$  it only remains the evaluation of the corresponding large- $D$  behavior of the angular part  $R_q[\mathcal{Y}_{l,\{\mu\}}]$  which will be done in the following.

## 2. Angular Rényi entropy

Here we will effort to calculate the large- $D$  behavior of the angular part  $R_q[\mathcal{Y}_{l,\{\mu\}}]$  of the total position and momentum Rényi entropies defined by Eq. (24). Therein, according to (11) and (21), the Rényi-like functional  $\Lambda_{l,\{\mu\}}(\Omega_{D-1})$  of the hyperspherical harmonics can be expressed as

$$\begin{aligned} \Lambda_{l,\{\mu\}}(\Omega_{D-1}) &= \int_{S^{D-1}} |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^{2q} d\Omega_{D-1} \\ &= \mathcal{N}_{l,\{\mu\}}^{2q} \int_{S^{D-1}} \prod_{j=1}^{D-2} [C_{\mu_j-\mu_{j+1}}^{(\alpha_j+\mu_{j+1})}(\cos \theta_j)]^{2q} (\sin \theta_j)^{2q\mu_{j+1}} d\Omega_{D-1} \\ &= 2\pi \mathcal{N}_{l,\{\mu\}}^{2q} \prod_{j=1}^{D-2} \int_0^\pi [C_{\mu_j-\mu_{j+1}}^{(\alpha_j+\mu_{j+1})}(\cos \theta_j)]^{2q} (\sin \theta_j)^{2q\mu_{j+1}+2\alpha_j} d\theta_j \end{aligned}$$

where the normalization constant  $\mathcal{N}_{l,\{\mu\}}$  is given by (12). Moreover, note that the integrals within the product are Rényi-like functionals of Gegenbauer polynomials of the type considered in Theorem 2 (see Appendix B).

To calculate the dominant term of  $\Lambda_{l,\{\mu\}}(\Omega_{D-1})$  at large  $D$  we use the Theorem 2 at zeroth-order

or, what is equivalent, we use the following limiting expressions of the Gegenbauer polynomials to monomials (see [41], Eq. 18.6.4)

$$\lim_{\alpha' \rightarrow \infty} (2\alpha')^{-k} \mathcal{C}_k^{(\alpha')} (x) = \frac{x^k}{k!}, \quad (33)$$

which allows us to find

$$\begin{aligned} \Lambda_{l, \{\mu\}}(\Omega_{D-1}) &\sim 2\pi \mathcal{N}_{l, \{\mu\}}^{2q} \prod_{j=1}^{D-2} \frac{[2(\alpha_j + \mu_{j+1})]^{2q(\mu_j - \mu_{j+1})}}{[\Gamma(\mu_j - \mu_{j+1} + 1)]^{2q}} \int_0^\pi (\cos \theta_j)^{2q(\mu_j - \mu_{j+1})} (\sin \theta_j)^{2(q\mu_{j+1} + \alpha_j)} d\theta_j \\ &= 2\pi \mathcal{N}_{l, \{\mu\}}^{2q} \prod_{j=1}^{D-2} \frac{[2(\alpha_j + \mu_{j+1})]^{2q(\mu_j - \mu_{j+1})}}{[\Gamma(\mu_j - \mu_{j+1} + 1)]^{2q}} B\left(q\mu_{j+1} + \frac{1}{2} + \alpha_j, q(\mu_j - \mu_{j+1}) + \frac{1}{2}\right) \\ &= (2\pi)^{1+(1-D)q} \left( \prod_{j=1}^{D-2} \frac{\Gamma(q(\mu_j - \mu_{j+1}) + \frac{1}{2})}{\Gamma(\mu_j - \mu_{j+1} + 1)^q} \right) \left( \prod_{j=1}^{D-2} (\alpha_j + \mu_j)(\alpha_j + \mu_{j+1})^{2(\mu_j - \mu_{j+1})} \right)^q \\ &\quad \times \left( \prod_{j=1}^{D-2} \frac{\Gamma(\alpha_j + q\mu_{j+1} + \frac{1}{2})}{\Gamma(\alpha_j + q\mu_j + 1)} \right) \left( \prod_{j=1}^{D-2} 4^{q(\alpha_j + \mu_j)} \frac{\Gamma(\alpha_j + \mu_{j+1})^{2q}}{\Gamma(2\alpha_j + \mu_{j+1} + \mu_j)^q} \right). \end{aligned} \quad (34)$$

Further algebraic manipulations, which are detailed in Appendix C, have allowed us to obtain that

$$\begin{aligned} \Lambda_{l, \{\mu\}}(\Omega_{D-1}) &\sim \left( 2^{1-q} \frac{\Gamma(1 + q\mu_{D-1})}{\Gamma(1 + \mu_{D-1})^q} \tilde{\mathcal{M}}(D, q, \{\mu\}) \right) \\ &\quad \times \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \pi^{\frac{D}{2}(1-q)} \frac{\Gamma(\frac{D}{2} + l)^q}{\Gamma(\frac{D}{2} + ql)} \right) \end{aligned} \quad (35)$$

where

$$\tilde{\mathcal{M}}(D, q, \{\mu\}) \equiv 4^{q(l - \mu_{D-1})} \pi^{1 - \frac{D}{2}} \prod_{j=1}^{D-2} \frac{\Gamma(q(\mu_j - \mu_{j+1}) + \frac{1}{2})}{\Gamma(\mu_j - \mu_{j+1} + 1)^q} \quad (36)$$

and

$$\tilde{\mathcal{E}}(D, \{\mu\}) \equiv \prod_{j=1}^{D-2} \frac{(\alpha_j + \mu_{j+1})^{2(\mu_j - \mu_{j+1})}}{(2\alpha_j + 2\mu_{j+1})_{\mu_j - \mu_{j+1}}} \frac{1}{(\alpha_j + \mu_{j+1})_{\mu_j - \mu_{j+1}}}. \quad (37)$$

Note that  $\tilde{\mathcal{E}} = \tilde{\mathcal{M}} = 1$  for any configuration with  $\mu_1 = \mu_2 = \dots = \mu_{D-1}$ . Finally, as explained in Appendix C, we have the following expression

$$\begin{aligned} R_q[\mathcal{Y}_{l, \{\mu\}}] &\sim \frac{1}{1-q} \log \left( \frac{\Gamma(\frac{D}{2} + l)^q}{\Gamma(\frac{D}{2} + ql)} \right) + \frac{D}{2} \log \pi \\ &\quad + \frac{1}{1-q} \log \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \frac{\Gamma(1 + q\mu_{D-1})}{\Gamma(1 + \mu_{D-1})^q} 2^{1-q} \right) \\ &\sim -\log \left( \Gamma \left( \frac{D}{2} \right) \right) + \frac{D}{2} \log \pi + \frac{1}{1-q} \log \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \frac{\Gamma(1 + q\mu_{D-1})}{\Gamma(1 + \mu_{D-1})^q} 2^{1-q} \right) \\ &\sim -\frac{D}{2} \log D + \frac{D}{2} \log(2\pi e) + \frac{1}{2} \log D + \frac{1}{1-q} \log \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \frac{\Gamma(1 + q\mu_{D-1})}{\Gamma(1 + \mu_{D-1})^q} \left( \frac{\pi}{2} \right)^{\frac{q-1}{2}} \right) \end{aligned} \quad (38)$$



for the angular Rényi entropy of the generic hydrogenic state with hyperquantum numbers  $(l, \{\mu\})$ , which holds for every non-negative  $q \neq 1$ .

For completeness, we will determine this asymptotic behavior in a more complete manner for some physically-relevant and experimentally accessible states like the (*ns*) and circular ones, which are described by the hyperquantum numbers  $(n, l = 0, \{\mu\} = \{0\})$  and  $(n, l = n - 1, \{\mu\} = \{n - 1\})$ , respectively. First we obtain from (34) the following values

$$\Lambda_{0,\{0\}}(\Omega_{D-1}) \sim 2\pi \mathcal{N}_{0,\{0\}}^{2q} \prod_{j=1}^{D-2} \frac{\Gamma(\frac{1}{2})\Gamma(\alpha_j + \frac{1}{2})}{\Gamma(\alpha_j + 1)} = \left( \frac{2\pi^{\frac{D}{2}}}{\Gamma(\frac{D}{2})} \right)^{1-q} \quad (39)$$

and

$$\begin{aligned} \Lambda_{n-1,\{n-1\}}(\Omega_{D-1}) &\sim 2\pi \mathcal{N}_{n-1,\{n-1\}}^{2q} \prod_{j=1}^{D-2} \frac{\Gamma(\frac{1}{2})\Gamma(\alpha_j + q(n-1)\frac{1}{2})}{\Gamma(\alpha_j + q(n-1) + 1)} \\ &= \left( 2\pi^{\frac{D}{2}} \right)^{1-q} \prod_{j=1}^{D-2} \left( \frac{\Gamma(\alpha_j + n)}{\Gamma(\alpha_j + n - \frac{1}{2})} \right)^q \frac{\Gamma(\alpha_j + q(n-1) + \frac{1}{2})}{\Gamma(\alpha_j + q(n-1) + 1)} \\ &= \left( \frac{1}{2\pi^{\frac{D}{2}}} \right)^{q-1} \frac{\left( (n)_{\frac{D}{2}-1} \right)^q}{(1 + q(n-1))_{\frac{D}{2}-1}}, \end{aligned} \quad (40)$$

respectively. Note that  $(x)_a = \frac{\Gamma(x+a)}{\Gamma(x)}$  is the well-known Pochhammer symbol. Then, from Eqs. (24), (39) and (40), we have that the angular part of the Rényi entropy at large  $D$  is given by

$$R_q[\mathcal{Y}_{0,\{0\}}] \sim \log \left( \frac{2\pi^{\frac{D}{2}}}{\Gamma(\frac{D}{2})} \right) \quad (41)$$

and

$$R_q[\mathcal{Y}_{n-1,\{n-1\}}] \sim \frac{1}{1-q} \log \left( \left( \frac{1}{2\pi^{\frac{D}{2}}} \right)^{q-1} \frac{\left( (n)_{\frac{D}{2}-1} \right)^q}{(1 + q(n-1))_{\frac{D}{2}-1}} \right) \quad (42)$$

for the (*ns*) and circular states, respectively. Note that for very large  $D$  the dominant term of the angular Rényi entropy of these two classes of physical states is the same; namely,  $-\log(\Gamma(\frac{D}{2})) + \frac{D}{2} \log \pi$ . Moreover and most interesting: this is true for any hydrogenic state by taking into account the general expression (38). This observation allows us to conjecture the expression

$$S[\mathcal{Y}_{l,\{\mu\}}] \sim -\log \left( \Gamma \left( \frac{D}{2} \right) \right) + \frac{D}{2} \log \pi. \quad (43)$$

for the large- $D$  behavior of the angular Shannon entropy of the hydrogenic states.

## 3. Total position Rényi entropy

To obtain the total Rényi entropy  $R_q[\rho_{n,l,\{\mu\}}]$  in position space for a general  $(n, l, \{\mu\})$ -state, according to (22), we have to sum up the radial and angular contributions given by (31) and (38), respectively. Then, we obtain that

$$\begin{aligned}
 R_q[\rho_{n,l,\{\mu\}}] &\sim \log\left(\frac{D^{2D}}{\Gamma\left(\frac{D}{2}\right)}\right) + D \log\left(\frac{q^{\frac{1}{q-1}}\sqrt{\pi}}{4Ze}\right) + \frac{q(n-l-\frac{1}{2})-\frac{1}{2}}{1-q} \log D \\
 &\quad + \frac{1}{1-q} \log\left(\tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \mathcal{F}(n, l, q) \frac{\Gamma(1+q\mu_{D-1})}{\Gamma(1+\mu_{D-1})^q} \left(\frac{\pi}{2}\right)^{\frac{q-1}{2}}\right) \\
 &\sim \frac{3}{2}D \log D + D \log\left(\frac{q^{\frac{1}{q-1}}\sqrt{\pi}}{Z} \sqrt{8e}\right) + \frac{q(n-l-1)}{1-q} \log D \\
 &\quad + \frac{1}{1-q} \log\left(\tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \mathcal{F}(n, l, q) \frac{\Gamma(1+q\mu_{D-1})}{\Gamma(1+\mu_{D-1})^q} \left(\frac{\pi}{2}\right)^{\frac{q-1}{2}}\right)
 \end{aligned} \tag{44}$$

which holds for every non-negative  $q \neq 1$ . Now, for completeness we calculate this quantity in an explicit manner for the  $(ns)$  and circular states, which both of them include the ground state. For the  $(ns)$  and circular states we have the asymptotical expressions

$$R_q[\rho_{n,0,\{0\}}] \sim \log\left(\frac{D^{2D}}{\Gamma\left(\frac{D}{2}\right)}\right) + D \log\left(\frac{q^{\frac{1}{q-1}}\sqrt{\pi}}{4Ze}\right) + \frac{q(n-1)}{1-q} \log D + \frac{1}{1-q} \log(\mathcal{F}(n, 0, q)) - \frac{1}{2} \log \frac{\pi}{2}, \tag{45}$$

(with  $\mathcal{F}(n, 0, q) = \frac{|q-1|^{2(n-1)q}}{(2\pi)^{\frac{1}{2}(q-1)}[(n-1)!]^q}$ ) and

$$\begin{aligned}
 R_q[\rho_{n,n-1,\{n-1\}}] &\sim \frac{1}{1-q} \log\left(\frac{\left(\binom{n}{\frac{D}{2}-1}\right)^q}{(1+q(n-1))^{\frac{D}{2}-1}}\right) + 2D \log D \\
 &\quad + D \log\left(\frac{q^{\frac{1}{q-1}}\sqrt{\pi}}{4Ze}\right) + \frac{1}{1-q} \log\left(\mathcal{F}(n, n-1, q) \frac{\Gamma(1+q(n-1))}{\Gamma(n)^q}\right) - \frac{1}{2} \log \frac{\pi}{2} \\
 &\sim \log\left(\frac{D^{2D}}{\Gamma\left(\frac{D}{2}\right)}\right) + D \log\left(\frac{q^{\frac{1}{q-1}}\sqrt{\pi}}{4Ze}\right) + \frac{1}{1-q} \log\left(\frac{\Gamma(1+q(n-1))}{q^{2q(n-1)}\Gamma(n)^q}\right) + 2n + \log 2 - 3,
 \end{aligned} \tag{46}$$

respectively. Most interesting, we realize that the large- $D$  behavior of the total Rényi entropy in the position space for the hydrogenic ground state  $R_q[\rho_{1,0,\{0\}}]$  is given by the last expression above indicated.

Finally, from (44) one can conjecture that the Shannon entropy  $S[\rho_{n,l,\{\mu\}}]$  in position space for a general  $(n, l, \{\mu\})$ -state is given by

$$\begin{aligned} S[\rho_{n,l,\{\mu\}}] &\sim \log \left( \frac{D^{2D}}{\Gamma\left(\frac{D}{2}\right)} \right) + D \log \left( \frac{\sqrt{\pi}}{4Z} \right) \\ &\sim \frac{3}{2}D \log D + D \log \left( \frac{\sqrt{e\pi}}{\sqrt{8Z}} \right) \end{aligned} \quad (47)$$

but this is somehow risky because of the unknown  $(q \rightarrow 1)$ -behavior of the angular part, coming from the second line of Eq. (44).

### B. Rényi entropy in momentum space

Let us now determine the momentum Rényi entropy of the probability density  $\gamma_{n,l,\{\mu\}}(\vec{p})$  given by (18), which is defined as

$$R_q[\gamma_{n,l,\{\mu\}}] = \frac{1}{1-q} \log W_q[\gamma_{n,l,\{\mu\}}]; \quad 0 < q < \infty, \quad q \neq 1, \quad (48)$$

where

$$W_q[\gamma_{n,l,\{\mu\}}] = \int_{\mathbb{R}^D} [\gamma_{n,l,\{\mu\}}(\vec{p})]^q d\vec{p} \quad (49)$$

denote the momentum entropic moments. Then, operating in a similar way as in position space, we obtain that

$$R_q[\gamma_{n,l,\{\mu\}}] = R_q[\gamma_{n,l}] + R_q[\mathcal{Y}_{l,\{\mu\}}], \quad (50)$$

where  $R_q[\gamma_{n,l}]$  denotes the radial part

$$R_q[\gamma_{n,l}] = \frac{1}{1-q} \log \int_0^\infty [\mathcal{M}_{n,l}(p)]^{2q} p^{D-1} dp, \quad (51)$$

and  $R_q[\mathcal{Y}_{l,\{\mu\}}]$  denotes the angular part given by (24).

Since the angular entropy  $R_q[\mathcal{Y}_{l,\{\mu\}}]$  has been already calculated and discussed, it only remains to determine at large  $D$  the radial Rényi entropy  $R_q[\gamma_{n,l}]$ , given by (51), being all the hyperquantum numbers fixed.

## 1. Radial momentum Rényi entropy

To find the radial momentum Rényi entropy (51) at  $D \gg 1$ , we first rewrite for convenience the radial part of the wave function,  $\mathcal{M}_{n,l}(p)$ , given by (18) as

$$\begin{aligned} \mathcal{M}_{n,l}(p) &= \left(\frac{\eta}{Z}\right)^{\frac{D}{2}} (1+y)^{\frac{3}{2}} \left(\frac{1+y}{1-y}\right)^{\frac{D-2}{4}} \sqrt{w_\alpha(y)} \tilde{\mathcal{C}}_{n-l-1}^{(\alpha)}(y) \\ &= \left(\frac{\eta}{Z}\right)^{\frac{D}{2}} A(n, l; D)^{\frac{1}{2}} (1-y)^{\frac{1}{2}} (1+y)^{\frac{D+l+1}{2}} \mathcal{C}_{n-l-1}^{(l+\frac{D-1}{2})}(y), \end{aligned} \quad (52)$$

with  $y = \frac{1-\eta^2\tilde{p}^2}{1+\eta^2\tilde{p}^2}$ ,  $\tilde{p} = p/Z$ ,  $\alpha = l + \frac{D-1}{2}$ , and  $\tilde{\mathcal{C}}_{n-l-1}^{(\alpha)}(x)$  denotes the orthonormal Gegenbauer polynomials with respect to the weight function  $w_\alpha(x) = (1-x^2)^{\alpha-\frac{1}{2}}$ , so that  $\tilde{\mathcal{C}}_{n-l-1}^{(l+\frac{D-1}{2})}(x) = A(n, l; D)^{\frac{1}{2}} \mathcal{C}_{n-l-1}^{(l+\frac{D-1}{2})}(x)$ , where the constant

$$A(n, l; D) = \frac{(n-l-1)!(n+\frac{D-3}{2})[\Gamma(l+\frac{D-1}{2})]^2}{2^{2-2l-D}\pi\Gamma(n+l+D-2)}. \quad (53)$$

The radial momentum Rényi entropy (51) together with (52) can be expressed as

$$R_q[\mathcal{M}_{n,l}] = -D \log \frac{\eta}{Z} + \frac{1}{1-q} \{q \log A(n, l; D) + \log I_{n,l}(q, D)\} \quad (54)$$

and the following Rényi-like functional of Gegenbauer polynomials

$$I_{n,l}(q, D) = \int_{-1}^1 (1-y)^{lq-1+\frac{D}{2}} (1+y)^{(l+1)q-1+(q-\frac{1}{2})D} [\mathcal{C}_{n-l-1}^{(l+\frac{D-1}{2})}(y)]^{2q} dy. \quad (55)$$

It only remains to find the large- $D$  behavior of the two terms in (54) when  $(n, l, q)$  are fixed. The asymptotic estimate of  $A(n, l; D)$  turns out to be given by

$$A(n, l; D) \sim \frac{\Gamma(n-l)}{\sqrt{2\pi}} D^{l-n+\frac{3}{2}}. \quad (56)$$

On the other hand, the behavior of  $I_{n,l}(q, D)$  at large  $D$  can be obtained from Theorem 2 (see Appendix B) by studying the large- $\alpha$  behavior of the integral  $J_2(a, b, c, d, \kappa, m'; \alpha)$  with the parameters  $a = l(q-1) - \frac{1}{2}$ ,  $b = l(1-q) + 2q - \frac{3}{2}$ ,  $c = 1$ ,  $d = 2q - 1$ ,  $\kappa = 2q$ ,  $m' = n - l - 1$  and  $\alpha = l + \frac{D-1}{2}$ . Note that the condition  $c < d$  of the theorem provokes that  $q > 1$ . We have found that

$$\begin{aligned} I_{n,l}(q, D) &\sim \left(\frac{(2q-1)^{2q-1}}{q^{2q}}\right)^{\frac{D}{2}} \left(\frac{\Gamma(\frac{D}{2} + n - \frac{3}{2})}{\Gamma(\frac{D}{2} + l - \frac{1}{2})}\right)^{2q} (D+2l-1)^{-\frac{1}{2}} Q_0(n, l, q) \\ &\sim \left(\frac{(2q-1)^{2q-1}}{q^{2q}}\right)^{\frac{D}{2}} \left(\frac{D}{2}\right)^{2q(n-l-1)} (D+2l-1)^{-\frac{1}{2}} Q_0(n, l, q) \\ &\sim \left(\frac{(2q-1)^{2q-1}}{q^{2q}}\right)^{\frac{D}{2}} D^{2q(n-l-1)-\frac{1}{2}} \frac{Q_0(n, l, q)}{4q^{n-l-1}} \end{aligned} \quad (57)$$

for  $q > 1$  and where  $Q_0(q)$  is given by

$$Q_0(q, n, l) = \frac{\sqrt{2\pi} 4^{q(n-l-1)} (2q-1)^{q(l+1)-\frac{1}{2}} (q-1)^{2q(n-l-1)}}{\Gamma(n-l)^{2q} q^{q(2n-1)-\frac{1}{2}}}. \quad (58)$$

Using (56) and (57) we obtain the following behavior at large  $D$  for the radial part of the momentum Rényi entropy:

$$\begin{aligned} R_q[\mathcal{M}_{n,l}] &\sim -D \log\left(\frac{\eta}{Z}\right) + \frac{D}{1-q} \log \sqrt{\frac{(2q-1)^{2q-1}}{q^{2q}} + \frac{q(n-l-\frac{1}{2}) - \frac{1}{2}}{1-q} \log D} \\ &\quad + \frac{1}{1-q} \log \bar{Q}_0(q, n, l) \\ &\sim -D \log\left(\frac{D}{2Z}\right) + \frac{D}{1-q} \log \sqrt{\frac{(2q-1)^{2q-1}}{q^{2q}} + \frac{q(n-l-\frac{1}{2}) - \frac{1}{2}}{1-q} \log D} \\ &\quad + \frac{1}{1-q} \log \bar{Q}_0(q, n, l) \end{aligned} \quad (59)$$

with  $\bar{Q}_0(q, n, l) = \frac{\Gamma(n-l)^q}{(2\pi)^{\frac{q}{2}} 4^{q(n-l-1)}} Q_0(q, n, l) = \frac{(2\pi)^{\frac{1-q}{2}} (2q-1)^{q(l+1)-\frac{1}{2}} (q-1)^{2q(n-l-1)}}{\Gamma(n-l)^q q^{q(2n-1)-\frac{1}{2}}}$  (where we have used in the second expression that  $\eta = n + \frac{D-3}{2} \sim \frac{D}{2}$  for fixed  $n$ ) for a general  $(n, l)$ -state. Note that in the limit  $q \rightarrow 1$  this expression suggests that the behavior of the radial Shannon entropy in the momentum space can be conjectured at large  $D$  as

$$S[\mathcal{M}_{n,l}] \sim -D \log\left(\frac{D}{2Z}\right). \quad (60)$$

Then, according to Eq. (50), to fix the large  $D$ -behavior of the total Rényi entropy  $R_p[\gamma_{n,l,\{\mu\}}]$  it only remains the evaluation of the corresponding behavior of the angular part  $R_p[\mathcal{Y}_{l,\{\mu\}}]$  which was found in (38).

## 2. Total momentum Rényi entropy

To obtain the total Rényi entropy in momentum space for a general  $(n, l, \{\mu\})$ -state of a large-dimensional hydrogenic system we have to sum up the radial and angular contributions, given by (50), and then to take into account the final expressions (59) and (38) for these contributions.

Then, it follows the expression

$$\begin{aligned}
 R_q[\gamma_{n,l,\{\mu\}}] &\sim -\log\left(\frac{\eta^D \Gamma\left(\frac{D}{2}\right)}{Z^D}\right) + D \log\left(\sqrt{\pi} \left(\frac{(2q-1)^{2q-1}}{q^{2q}}\right)^{\frac{1}{2-2q}}\right) \\
 &\quad + \frac{q(n-l-\frac{1}{2})-\frac{1}{2}}{1-q} \log D + \frac{1}{1-q} \log\left(\tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \bar{Q}_0(q, n, l) \pi^{\frac{q-1}{2}}\right) \\
 &\sim -\frac{3}{2} D \log D + D \log\left(Z \sqrt{8e\pi} \left(\frac{(2q-1)^{2q-1}}{q^{2q}}\right)^{\frac{1}{2-2q}}\right) \\
 &\quad + \frac{q(n-l-1)}{1-q} \log D + \frac{1}{1-q} \log\left(\tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \bar{Q}_0(q, n, l) \pi^{\frac{q-1}{2}}\right),
 \end{aligned} \tag{61}$$

(with  $q \neq 1$  and  $\eta \sim \frac{D}{2}$ ) for the large- $D$  behavior of the total momentum Rényi entropy of the generic hydrogenic state  $(n, l, \{\mu\})$ , where the symbols  $\tilde{\mathcal{M}}(D, q, \{\mu\})$  and  $\tilde{\mathcal{E}}(D, \{\mu\})$  are defined in Eqs. (36) and (37), respectively. For completeness and illustration, let us give in a more complete manner the behavior of this quantity at  $D \gg 1$  for some particular quantum states such as the ( $ns$ ) and circular states. For the ( $ns$ )-states we found

$$\begin{aligned}
 R_q[\gamma_{n,0,\{0\}}] &\sim -\frac{3}{2} D \log D + D \log\left(Z \sqrt{8e\pi} \left(\frac{(2q-1)^{2q-1}}{q^{2q}}\right)^{\frac{1}{2-2q}}\right) \\
 &\quad + \frac{q(n-1)}{1-q} \log D + \frac{1}{1-q} \log\left(\bar{Q}_0(q, n, 0) \pi^{\frac{q-1}{2}}\right)
 \end{aligned} \tag{62}$$

with

$$\bar{Q}_0(q, n, 0) = \frac{(2\pi)^{\frac{1-q}{2}} (2q-1)^{q-\frac{1}{2}} (q-1)^{2q(n-1)}}{\Gamma(n)^q q^{q(2n-1)-\frac{1}{2}}}. \tag{63}$$

And for the circular states we obtained the following large- $D$  behavior

$$\begin{aligned}
 R_q[\gamma_{n,n-1,\{n-1\}}] &\sim -\frac{3}{2} D \log D + D \log\left(Z \sqrt{8e\pi} \left(\frac{(2q-1)^{2q-1}}{q^{2q}}\right)^{\frac{1}{2-2q}}\right) \\
 &\quad + \frac{1}{1-q} \log\left(\bar{Q}_0(q, n, n-1) \pi^{\frac{q-1}{2}}\right)
 \end{aligned} \tag{64}$$

with

$$\bar{Q}_0(q, n, n-1) = (2\pi)^{\frac{1-q}{2}} \frac{(2q-1)^{qn-\frac{1}{2}}}{q^{q(2n-1)-\frac{1}{2}}}. \tag{65}$$

Note now that either from (62) or from (64) with  $n = 1$  we have the following large- $D$  behavior

$$R_q[\gamma_{1,0,\{0\}}] \sim -\frac{3}{2}D \log D + D \log \left( Z\sqrt{8e\pi} \left( \frac{(2q-1)^{2q-1}}{q^{2q}} \right)^{\frac{1}{2-2q}} \right) + \frac{1}{1-q} \log \left( \bar{Q}_0(q, 1, 0) \pi^{\frac{q-1}{2}} \right) \quad (66)$$

with  $q \neq 1$  and  $\bar{Q}_0(q, 1, 0) = (2\pi)^{\frac{1-q}{2}} \left( 2 - \frac{1}{q} \right)^{q-\frac{1}{2}}$  for the total momentum Rényi entropy of the ground hydrogenic state.

Finally, from (61) one can conjecture that the Shannon entropy  $S[\rho_{n,l,\{\mu\}}]$  in momentum space for a general  $(n, l, \{\mu\})$ -state is given by

$$S[\gamma_{n,l,\{\mu\}}] \sim -\frac{3}{2}D \log D + D \log \left( Z\sqrt{8e\pi} \right) \quad (67)$$

in the limiting case  $q \rightarrow 1$ .

### C. Position-momentum Rényi-entropy-based uncertainty sum

From Eqs. (44) and (61) we can obtain the dominant term for the joint position-momentum Rényi-entropy-based uncertainty sum of a large-dimensional hydrogenic system for a pair of parameters  $p$  and  $q$  which fulfill the Holder conjugacy relation  $\frac{1}{p} + \frac{1}{q} = 2$ . We found that

$$R_q[\rho_{n,l,\{\mu\}}] + R_p[\gamma_{n,l,\{\mu\}}] \sim D \log \left[ \pi \left( \frac{(2p-1)^{(2p-1)}}{p^{2p}} \right)^{\frac{1}{2-2p}} q^{\frac{1}{q-1}} \right] = D \log \left[ 2\pi (2p)^{\frac{1}{2p-2}} (2q)^{\frac{1}{2q-2}} \right], \quad q \neq 1 \quad (68)$$

for all  $(n, l, \{\mu\})$ -states, which saturates the known position-momentum Rényi-entropy-based uncertainty relation [38–40]. Note that out of the so called conjugacy curve (i.e., for arbitrary positive pairs of values of  $p$  and  $q$ ), there is a dependence at second order on the quantum numbers  $n$  and  $l$ ; this dependence just disappears onto the conjugation line. A more detailed study of this behaviour out of the conjugacy curve remain as an open problem. Finally, the conjectured expressions for Shannon entropy in both spaces (47), (67) allows one to write

$$S[\rho_{n,l,\{\mu\}}] + S[\gamma_{n,l,\{\mu\}}] \sim D \log [2\pi e] \quad (69)$$

which saturates the general Bialynicki-Birula-Mycielski entropic relation [35, 38].

#### IV. CONCLUSIONS

In this work we have determined the large- $D$  behavior of the position and momentum Rényi entropies of the  $D$ -dimensional hydrogenic states at large  $D$  in terms of the state's hyperquantum numbers and the nuclear charge  $Z$  of the system. We have used a recent constructive methodology which allows for the calculation of some Rényi-like integral functionals of Laguerre  $\mathcal{L}_k^{(\alpha)}(x)$  and Gegenbauer  $\mathcal{C}_k^{(\alpha'')}(x)$  polynomials with a fixed degree  $k$  and large values of the parameters  $\alpha$  and  $\alpha''$ . This has been possible because the hydrogenic states are controlled by the Laguerre and Gegenbauer polynomials in position space, and by the Gegenbauer polynomials in momentum space, keeping in mind that the hyperspherical harmonics (which determine the angular part of the wave functions in the two conjugated spaces) can be expressed in terms of the latter polynomials. Then, simple expressions of these quantities for some specific classes of hydrogenic states ( $ns$  and circular states), which include the ground state, are given. Moreover, as a byproduct, our results reach the saturation of the known position-momentum Rényi-entropy-based uncertainty relations. To this respect we should keep in mind that we are assuming that the dimensionality is very large and the hyperquantum numbers are small. The exceptional case when both dimensionality and hyperquantum numbers are simultaneously large has not yet been explored; in particular, we cannot assure saturation.

We should highlight that to find the Shannon entropies of the large-dimensional hydrogenic systems have not yet been possible with the present methodology, although the dominant term has been conjectured. A rigorous proof remains open.

Finally, let us mention that it would be very relevant for many quantum-mechanical problems other than the hydrogenic ones (e.g., the harmonic systems) the determination of the behavior of integral functionals of Rényi and Shannon types for hypergeometric polynomials other than the Laguerre and Gegenbauer ones at large values of the polynomials' parameters and fixed degrees. This is yet another open problem for the future.

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### Appendix A: Rényi-like functionals of Laguerre polynomials with large parameters

In this appendix the asymptotics ( $\alpha \rightarrow \infty$ ) of some Rényi-like functionals of the Laguerre polynomials is given by means of the following theorem which has been recently found [43] (see also [44, 45]). Herein, the involved parameters are just algebraic numbers without any quantum interpretation.

**Theorem 1.** *The Rényi-like functional of the Laguerre polynomials  $\mathcal{L}_m^{(\alpha)}(x)$  given by*

$$J_1(\sigma, \lambda, \kappa, m; \alpha) = \int_0^\infty x^{\alpha+\sigma-1} e^{-\lambda x} \left| \mathcal{L}_m^{(\alpha)}(x) \right|^\kappa dx, \quad (\text{A1})$$

(with  $\sigma$  real,  $0 < \lambda \neq 1$ ,  $\kappa > 0$ ) has the following ( $\alpha \rightarrow \infty$ )-asymptotic behavior

$$J_1(\sigma, \lambda, \kappa, m; \alpha) \sim \alpha^{\alpha+\sigma} e^{-\alpha} \lambda^{-\alpha-\sigma-\kappa m} |\lambda - 1|^{\kappa m} \sqrt{\frac{2\pi}{\alpha}} \frac{\alpha^{\kappa m}}{(m!)^\kappa} \sum_{j=0}^\infty \frac{D_j}{\alpha^j}, \quad (\text{A2})$$

with the first coefficients  $D_0 = 1$  and

$$D_1 = \frac{1}{12(\lambda - 1)^2} \left( 1 - 12\kappa m \sigma \lambda + 6\sigma^2 \lambda^2 - 12\sigma^2 \lambda - 6\sigma \lambda^2 + 12\sigma \lambda + \right. \\ \left. 6\kappa^2 m^2 + 12\kappa m \sigma - 12\kappa m^2 \lambda - 12\kappa m \lambda + 6\kappa m \lambda^2 + \right. \\ \left. 6\kappa m^2 \lambda^2 + \lambda^2 + 6\sigma^2 - 2\lambda - 6\sigma + 6\kappa m^2 \right). \quad (\text{A3})$$

For the knowledge of the remaining coefficients and further details about the theorem, see [43].

### Appendix B: Rényi-like functionals of Gegenbauer polynomials with large parameters

In this appendix the asymptotics ( $\alpha \rightarrow \infty$ ) of some Rényi-like functionals of Gegenbauer polynomials is given by means of the following theorem which has been recently found [43] (see also [44, 45]). Herein, the involved parameters are just algebraic numbers without any quantum interpretation.

**Theorem 2.** Let  $a, b, c, d$ , and  $\kappa$  be positive real numbers,  $c < d$ , and  $m$  a positive natural number. Then, the Rényi-like functional of the Gegenbauer polynomials  $\mathcal{C}_m^{(\alpha)}(x)$  given by

$$J_2(a, b, c, d, \kappa, m; \alpha) = \int_{-1}^1 (1-x)^{c\alpha+a} (1+x)^{d\alpha+b} \left| \mathcal{C}_m^{(\alpha)}(x) \right|^\kappa dx \quad (\text{B1})$$

has the following asymptotics:

$$J_2(a, b, c, d, \kappa, m; \alpha) \sim e^{-\alpha\phi(x_m)} \sqrt{\frac{2\pi}{\alpha}} \frac{2^{\kappa m} ((\alpha)_m)^\kappa}{(m!)^\kappa} \sum_{k=0}^{\infty} \frac{D_k}{\alpha^k}, \quad \alpha \rightarrow \infty \quad (\text{B2})$$

where the coefficients  $D_k$  do not depend on  $\alpha$ . The first coefficient is given by

$$D_0 = a_1 \left( \frac{2c}{c+d} \right)^a \left( \frac{2d}{c+d} \right)^b \left( \frac{d-c}{c+d} \right)^{\kappa m}, \quad (\text{B3})$$

and the symbols  $x_m = (d-c)/(d+c)$ ,  $\phi(x_m) = -c \log \frac{2c}{c+d} - d \log \frac{2d}{c+d}$  and  $a_1 = 2\sqrt{\frac{cd}{(c+d)^3}}$ .

Moreover, if  $c = d$ , the corresponding Rényi-like functional

$$J_2(a, b, c, \kappa, m; \alpha) = \int_{-1}^1 (1-x)^a (1+x)^b e^{-\alpha\phi(x)} \left| \mathcal{C}_m^{(\alpha)}(x) \right|^\kappa dx, \quad (\text{B4})$$

has the asymptotic behavior

$$J_2(a, b, c, \kappa, m; \alpha) \sim \sqrt{\frac{\pi}{\alpha c}} \frac{(2\alpha)^m}{m!}, \quad \alpha \rightarrow \infty. \quad (\text{B5})$$

Finally, the asymptotics of the Rényi-like functional with  $c > d$  follows from the one with  $c < d$  by interchanging  $a$  and  $b$  and  $c$  and  $d$ . The case  $c > d$  is useful for the determination of the Rényi entropy of the large dimensional hydrogenic states in momentum space with  $q < 1$ . For further details of the theorem, see [43].

### Appendix C: Large- $D$ behavior of the angular Rényi factor $\Lambda_{l, \{\mu\}}(\Omega_{D-1})$

Here we gather the necessary steps to obtain the final asymptotical expression (35) for the angular Rényi factor  $\Lambda_{l, \{\mu\}}(\Omega_{D-1})$  from Eq. (34). First of all we have that since  $\alpha_{j+1} = \alpha_j - \frac{1}{2}$  one has that

$$\prod_{j=1}^{D-2} \frac{\Gamma(\alpha_j + q\mu_{j+1} + \frac{1}{2})}{\Gamma(\alpha_j + q\mu_j + 1)} = \frac{\Gamma(\alpha_{D-2} + q\mu_{D-1} + \frac{1}{2})}{\Gamma(\alpha_1 + q\mu_1 + 1)} = \frac{\Gamma(1 + q\mu_{D-1})}{\Gamma(\frac{D}{2} + ql)}$$

Then, we can express the product

$$\prod_{j=1}^{D-2} 4^{q(\alpha_j + \mu_j)} \frac{\Gamma(\alpha_j + \mu_{j+1})^{2q}}{\Gamma(2\alpha_j + \mu_{j+1} + \mu_j)^q} = \prod_{j=1}^{D-2} 4^{q(\alpha_j + \mu_j)} \frac{\Gamma(\alpha_j + \mu_{j+1})^{2q}}{\Gamma(2\alpha_j + 2\mu_{j+1})^q} \prod_{j=1}^{D-2} \frac{\Gamma(2\alpha_j + 2\mu_{j+1})^q}{\Gamma(2\alpha_j + \mu_{j+1} + \mu_j)^q},$$

whose first factor can be rewritten as

$$\begin{aligned} \prod_{j=1}^{D-2} 4^{q(\alpha_j + \mu_j)} \frac{\Gamma(\alpha_j + \mu_{j+1})^{2q}}{\Gamma(2\alpha_j + 2\mu_{j+1})^q} &= \prod_{j=1}^{D-2} 4^{q(\mu_j - \mu_{j+1})} (2\sqrt{\pi})^q \frac{\Gamma(\alpha_j + \mu_{j+1} + 1)^q}{\Gamma(\alpha_j + \mu_{j+1} + \frac{1}{2})^q} (\alpha_j + \mu_{j+1})^{-q} \\ &= 4^{q(l - \mu_{D-1})} (2\sqrt{\pi})^{q(D-2)} \frac{\Gamma(\frac{D}{2} + l)^q}{\Gamma(1 + \mu_{D-1})^q} \prod_{j=1}^{D-2} \frac{\Gamma(\alpha_j + \mu_{j+1} + 1)^q}{\Gamma(\alpha_j + \mu_j + 1)^q} (\alpha_j + \mu_{j+1})^{-q} \end{aligned}$$

Taking into account these previous observations, Eq. (34) becomes

$$\begin{aligned} \Lambda_{l, \{\mu\}}(\Omega_{D-1}) &\sim 2^{1-q} 4^{q(l - \mu_{D-1})} \pi^{1 - \frac{D}{2}} \mathcal{M}(D, q, \{\mu\}) (\mathcal{A}(D, \{\mu\}))^q \times \\ &\frac{\Gamma(\frac{D}{2} + l)^q}{\Gamma(\frac{D}{2} + ql)} \frac{\Gamma(1 + q\mu_{D-1})}{\Gamma(1 + \mu_{D-1})^q} \prod_{j=1}^{D-2} \frac{\Gamma(2\alpha_j + 2\mu_{j+1})^q}{\Gamma(2\alpha_j + \mu_{j+1} + \mu_j)^q} \frac{\Gamma(\alpha_j + \mu_{j+1} + 1)^q}{\Gamma(\alpha_j + \mu_j + 1)^q} \end{aligned} \quad (\text{C1})$$

where

$$\mathcal{M}(D, q, \{\mu\}) \equiv \prod_{j=1}^{D-2} \frac{\Gamma(q(\mu_j - \mu_{j+1}) + \frac{1}{2})}{\Gamma(\mu_j - \mu_{j+1} + 1)^q}$$

and

$$\mathcal{A}(D, \{\mu\}) \equiv \prod_{j=1}^{D-2} (\alpha_j + \mu_j) (\alpha_j + \mu_{j+1})^{2(\mu_j - \mu_{j+1}) - 1}$$

Now, for convenience we introduce the notation

$$\begin{aligned} \tilde{\mathcal{E}}(D, \{\mu\}) &\equiv \mathcal{A}(D, \{\mu\}) \times \prod_{j=1}^{D-2} \frac{(2\alpha_j + 2\mu_{j+1})_{\mu_j - \mu_{j+1}}^{-1}}{(\alpha_j + \mu_{j+1} + 1)_{\mu_j - \mu_{j+1}}} \\ &= \prod_{j=1}^{D-2} \frac{(\alpha_j + \mu_{j+1})^{2(\mu_j - \mu_{j+1})}}{(2\alpha_j + 2\mu_{j+1})_{\mu_j - \mu_{j+1}}} \frac{1}{(\alpha_j + \mu_{j+1})_{\mu_j - \mu_{j+1}}}, \end{aligned}$$

so that we have

$$\begin{aligned} \Lambda_{l, \{\mu\}}(\Omega_{D-1}) &\sim \left( \pi 2^{1-q+2q(l - \mu_{D-1})} \frac{\Gamma(1 + q\mu_{D-1})}{\Gamma(1 + \mu_{D-1})^q} \right) \\ &\times \left( \mathcal{M}(D, q, \{\mu\}) \frac{\tilde{\mathcal{E}}(D, \{\mu\})^q}{\pi^{q\frac{D}{2}}} \frac{\Gamma(\frac{D}{2} + l)^q}{\Gamma(\frac{D}{2} + ql)} \right) \end{aligned}$$

where the dominant factor is  $\frac{\Gamma(\frac{D}{2} + l)^q}{\Gamma(\frac{D}{2} + ql)} \sim \Gamma(\frac{D}{2})^{q-1}$ . Moreover we can still simplify this expression by the use of the notation  $\tilde{\mathcal{M}}$

$$\tilde{\mathcal{M}}(D, q, \{\mu\}) \equiv 4^{q(l - \mu_{D-1})} \pi^{1 - \frac{D}{2}} \mathcal{M}(D, q, \{\mu\})$$

to have  $\tilde{\mathcal{M}} \equiv 1$  for all configurations with  $\mu_1 = \mu_2 = \dots = \mu_{D-1}$ . Thus, we can finally obtain the searched expression (35); namely,

$$\begin{aligned} \Lambda_{l, \{\mu\}}(\Omega_{D-1}) &\sim \left( 2^{1-q} \frac{\Gamma(1 + q\mu_{D-1})}{\Gamma(1 + \mu_{D-1})^q} \right) \\ &\times \left( \tilde{\mathcal{M}}(D, q, \{\mu\}) \tilde{\mathcal{E}}(D, \{\mu\})^q \pi^{\frac{D}{2}(1-q)} \frac{\Gamma(\frac{D}{2} + l)^q}{\Gamma(\frac{D}{2} + ql)} \right) \end{aligned}$$

This expression together with (24) allow us to determine the dominant term of the angular Rényi entropy for fixed  $l$  as

$$R_q[\mathcal{Y}_{l,\{\mu\}}] \sim -\log\left(\Gamma\left(\frac{D}{2}\right)\right) + \frac{D}{2}\log\pi + \frac{1}{1-q}\log\left(\tilde{\mathcal{E}}(D,\{\mu\})^q\tilde{\mathcal{M}}(D,q,\{\mu\})\right) \quad (\text{C2})$$

(where the third term vanishes for  $\mu_1 = \mu_2 = \dots = \mu_{D-1}$ ) which corresponds to expression (38) with the values of  $\tilde{\mathcal{M}}(D,q,\{\mu\})$  and  $\tilde{\mathcal{E}}(D,\{\mu\})$  given above.

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## 2.3 General stationary states

In the two previous sections we have tackled, calculated and discussed the dominant term of the Rényi entropies of  $D$ -dimensional hydrogenic system for the two extreme high-energy (Rydberg) and high-dimensional (pseudo-classical) states, expressing them in a simple, closed form. In this Section we extend these previous achievements by determining the position and momentum Rényi entropies (with natural order  $q$  other than unity) *for all the discrete stationary states* of the multidimensional hydrogenic system directly in terms of the hyperquantum numbers which characterize the states, the nuclear charge and the space dimensionality. The found expressions are given through the not-so-well-known multivariate hypergeometric function of Lauricella and Srivastava-Daoust types evaluated at  $1/q$  and unity. Then, we also determine their associated uncertainty relations. To do that we use the Srivastava-Niukkanen linearization of Laguerre and Jacobi polynomials given by Theorems 1.5 and 1.6 of Section 1.3.

The following specific tasks have been done:

- Calculation of the position and momentum Rényi entropies for all quantum states of the multidimensional hydrogenic system from first principles; i.e., by means of the hyperquantum numbers, the Coulomb strength and the space dimensionality.
- Use of a recent methodology which allows to determine the involved integral functionals by taking into account the linearization formula and orthogonality conditions of the Laguerre and Jacobi polynomials; the latter ones are closely connected to the Gegenbauer polynomials which control the angular part of the wavefunctions in both conjugated spaces as well as the radial wavefunction in momentum space.
- Expression of the Rényi entropies in position and momentum spaces in a closed form by use of the hypergeometric function of Lauricella and Srivastava-Daoust types evaluated at  $1/q$  and unity, respectively.
- Determination of the corresponding global position-momentum uncertainty sum.

It remains as an open problem, the extension of this result to the limiting case  $q \rightarrow 1$ , which corresponds to the Shannon entropy, and the Rényi entropies for any real value of the parameter  $q$ . The latter requires a completely different approach, still unknown to the best of our knowledge.

These results are contained in the submitted paper [70] with coordinates: **Puertas-Centeno D.**, Toranzo I. V. and Dehesa J. S. *Analytical determination of position and momentum Rényi entropies for multidimensional hydrogenic systems*. Preprint UGR 2018, which is attached below.



# Rényi entropies for multidimensional hydrogenic systems in position and momentum spaces

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**Abstract.** The Rényi entropies of Coulomb systems  $R_p[\rho]$ ,  $0 < p < \infty$  are logarithms of power functionals of the electron density  $\rho(\vec{r})$  which quantify most appropriately the electron uncertainty and describe numerous physical observables. However, its analytical determination is a hard issue not yet solved except for the first lowest-lying energetic states of some specific systems. This is so even for the  $D$ -dimensional hydrogenic system, which is the main prototype of the multidimensional Coulomb many-body systems. Recently, the Rényi entropies of this system have been found in the two extreme high-energy (Rydberg) and high-dimensional (pseudo-classical) cases. In this work we determine the position and momentum Rényi entropies (with integer  $p$  greater than 1) for all the discrete stationary states of the multidimensional hydrogenic system directly in terms of the hyperquantum numbers which characterize the states, the nuclear charge and the space dimensionality. We have used a methodology based on linearization formulas for powers of the orthogonal Laguerre and Gegenbauer polynomials which control the hydrogenic states.

*Keywords:* Rényi entropies, multidimensional hydrogenic systems, Rényi entropies of multidimensional hydrogenic systems in position space, Rényi entropies of multidimensional hydrogenic systems in momentum space, Linearization of powers of orthogonal polynomials.

## 1. Introduction

In a seminal paper Alfréd Rényi [1] found axiomatically a set of mono-parametric information entropies of a probability density  $\rho(x)$  which includes the Shannon entropy as a limiting case. These Rényi quantities are logarithms of integral functionals of powers of  $\rho(x)$  (Yule-Sichel frequency moments [2, 3, 4]) appropriately renormalized to have an entropic character. They describe numerous spreading facets of the density and, moreover, completely characterize the density under certain conditions [5, 6]. Moreover, they are closely related to other information-theoretic quantities such as e.g., the Tsallis entropies [7] which play a very important role in systems with strong long-range correlations and nonextensive statistical mechanics [8, 9].

The properties of the Rényi entropies and their applications have been widely considered/applied (see e.g., [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26] and reviewed [27, 28, 29, 30] in a broad variety of fields ranging from applied mathematics, quantum physics, Rydberg physics, complexity theory to non-linear physics, option price calibration, nanotechnology and neuroscience. However, these quantities have not yet been exactly calculated except for a few one-dimensional exponential densities (see e.g., [17]) and some probability densities of a single-particle system moving in the elementary multidimensional quantum potentials of infinite well [18] and rigid rotator [25]) types. Moreover, the dominant term for the Rényi entropies of the multidimensional harmonic oscillator has been determined at the high-dimensional (pseudoclassical) and high-energy (Rydberg) limits [31, 32], and then the entropy values for both ground and excited oscillator-like states have been analytically calculated [33] in terms of the hyperquantum numbers and the oscillator strength.

Recently, the analytical determination of the Rényi entropies of the main prototype of the  $D$ -dimensional Coulomb many-body systems, the  $D$ -dimensional hydrogenic system, from first principles (i.e., in terms of the hyperquantum numbers of the state and the nuclear charge) has been undertaken [34, 35, 36]. This is relevant *per se* and for a reference point of view. The  $D$ -dimensional hydrogenic system is a negatively-charged particle moving in a space of  $D$  dimensions around a positively charged core which electromagnetically binds it in its orbit [37, 38, 39, 34, 40, 53, 42, 43]. This system allows for the modelling of numerous three-dimensional physical systems (e.g., hydrogenic atoms and ions, exotic atoms, antimatter atoms, Rydberg atoms) and a number of nanotechnological objects (quantum wells, wires and dots) and qubits which have been shown to be very useful in semiconductor physics [44, 45] and quantum technologies [46, 47], respectively. Moreover, it plays a crucial role for the interpretation of numerous phenomena of quantum cosmology [48] and quantum field theory [49, 50, 51]. In addition the  $D$ -dimensional hydrogenic wavefunctions have been used as complete orthonormal sets for many-body atomic and molecular problems [52, 53] in both position and momentum spaces.

The calculation of the hydrogenic Rényi entropies is a difficult task except for the lowest-lying energy states. This is because these quantities are described by means of some power or logarithmic functionals of the electron density, which cannot be easily handled in an analytical way nor numerically computed; the latter is basically because a naive numerical evaluation using quadratures is not convenient due to the increasing number of integrable singularities when the principal hyperquantum number  $n$  is increasing, which spoils any attempt to achieve reasonable accuracy even for rather small  $n$  [54]. Up until now, these quantities have been only calculated in a compact form [35, 55, 56] at the high-dimensional (pseudoclassical) and high-energy (Rydberg) limits by use of modern asymptotical techniques of the Laguerre and Gegenbauer polynomials which control the state's wavefunctions in position and momentum spaces [26, 57].

In this work we determine the Rényi entropies  $R_p[\rho]$  (with integer  $p$  greater than 1) for the electron density  $\rho(\vec{r})$  of all the discrete stationary states of the  $D$ -dimensional hydrogenic system directly in terms of the hyperquantum numbers which characterize the states, the nuclear charge and the space dimensionality  $D$ . The structure of the manuscript is the following. In Sec. 2 the notion of the  $p$ th-order Rényi entropy for a  $D$ -dimensional probability is given, and then the wavefunctions of the hydrogenic states in the  $D$ -dimensional configuration space are briefly described so as to express the associated probability densities. In Sec. 3 the position and momentum Rényi entropies are analytically determined by means of the little known polynomial linearization methodology of Srivastava-Niukkanen type [59, 60, 61, 62]. In Sec. 4 the specific values for the entropies of some particularly relevant hydrogenic states are given to illustrate the applicability of our procedure. Finally, some concluding remarks and open problems are given.

## 2. $D$ -dimensional hydrogenic system: An entropic view

In this section we briefly describe the quantum position and momentum probability setting of the  $D$ -dimensional hydrogenic system where the Rényi entropies are applied. For convenience we start with the definition of these entropies for a general multidimensional probability density, and then we give the known wavefunctions [37, 38, 39, 40] of the system in both position and momentum spaces as well as the corresponding quantum probability densities.

### 2.1. Rényi entropy

The Rényi entropies  $R_p[\rho]$  of a  $D$ -dimensional probability density  $\rho(\vec{r})$  are defined as

$$R_p[\rho] = \frac{1}{1-p} \ln W_p[\rho]; \quad 0 < p < \infty, \quad p \neq 1, \quad (1)$$

where  $W_p[\rho]$  denotes the entropic or Yule-Sichel frequency moment of order  $p$  of  $\rho(\vec{r})$  is given by

$$W_p[\rho] = \int_{\mathbb{R}^D} [\rho(\vec{r})]^p d\vec{r} = \|\rho\|_p^p; \quad p > 0, \quad (2)$$

where the position  $\vec{r} = (x_1, \dots, x_D)$  is given in hyperspherical units as  $(r, \theta_1, \theta_2, \dots, \theta_{D-1}) \equiv (r, \Omega_{D-1})$ ,  $\Omega_{D-1} \in S^{D-1}$ ; and the volume element is

$$d\vec{r} = r^{D-1} dr d\Omega_D, \quad d\Omega_{D-1} = \left( \prod_{j=1}^{D-2} \sin^{2\alpha_j} \theta_j d\theta_j \right) d\phi, \quad (3)$$

with  $2\alpha_j = D - j - 1$ . We have used  $r \equiv |\vec{r}| = \sqrt{\sum_{i=1}^D x_i^2} \in [0; +\infty)$  and  $x_i = r \left( \prod_{k=1}^{i-1} \sin \theta_k \right) \cos \theta_i$  for  $1 \leq i \leq D$  and with  $\theta_i \in [0; \pi)$ ,  $i < D - 1$ ,  $\theta_{D-1} \equiv \phi \in [0; 2\pi)$ . By convention  $\theta_D = 0$  and the empty product is the unity.

## 2.2. Hydrogenic system

The discrete stationary states of the  $D$ -dimensional hydrogenic system (i.e., a particle moving in the Coulomb potential  $V_D(r) = -\frac{Z}{r}$ , where  $Z$  denotes the nuclear charge; atomic units are used throughout the paper) are known to be expressed [38, 34] in position space by the energy eigenvalues

$$E = -\frac{Z^2}{2\eta^2}, \quad \eta = n + \frac{D-3}{2}; \quad n = 1, 2, 3, \dots, \quad (4)$$

and the associated eigenfunctions

$$\begin{aligned} \Psi_{n,l,\{\mu\}}(\vec{r}) &= N_{n,l} \left( \frac{r}{\lambda} \right)^l e^{-\frac{r}{2\lambda}} \mathcal{L}_{n-l-1}^{(2l+D-2)} \left( \frac{r}{\lambda} \right) \mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) \\ &= N_{\eta,l} \left[ \frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}} \right]^{1/2} \mathcal{L}_{\eta-L-1}^{(2L+1)}(\tilde{r}) \mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}), \end{aligned} \quad (5)$$

with

$$\begin{aligned} \eta &= n + \frac{D-3}{2}, \quad n = 1, 2, 3, \dots \\ L &= l + \frac{D-3}{2}, \quad l = 0, 1, 2, \dots \\ \tilde{r} &= \frac{r}{\lambda} \quad \text{with} \quad \lambda = \frac{\eta}{2Z}, \end{aligned} \quad (6)$$

The symbol  $\eta$  denotes the principal hyperquantum number of the state associated to the radial coordinate, and  $(l, \{\mu\}) \equiv (l \equiv \mu_1, \mu_2, \dots, \mu_{D-1})$  denote the orbital and magnetic hyperquantum numbers associated to the angular variables  $\Omega_{D-1} \equiv (\theta_1, \theta_2, \dots, \theta_{D-1})$ , which may take all values consistent with the inequalities  $l \equiv \mu_1 \geq \mu_2 \geq \dots \geq |\mu_{D-1}| \equiv |m| \geq 0$ . In addition,  $\omega_\alpha(x) = x^\alpha e^{-x}$ ,  $\alpha = 2l + D - 2$  is the weight function of the orthogonal and orthonormal Laguerre polynomials [63, 64] of degree  $n$  and parameter  $\alpha$ , here denoted by  $L_n^{(\alpha)}(x)$  and  $\hat{L}_n^{(\alpha)}(x)$ , respectively and

$$N_{n,l} = \lambda^{-\frac{D}{2}} \left( \frac{(\eta - L - 1)!}{2\eta(\eta + L)!} \right)^{\frac{1}{2}} \quad (7)$$

is the normalization constant which ensures the unit norm of the wavefunction. The angular part of the eigenfunctions is given by the hyperspherical harmonics as

$$\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) = \mathcal{N}_{l,\{\mu\}} e^{im\phi} \times \prod_{j=1}^{D-2} \mathcal{C}_{\mu_j - \mu_{j+1}}^{(\alpha_j + \mu_{j+1})}(\cos \theta_j) (\sin \theta_j)^{\mu_{j+1}} \quad (8)$$

where  $\mathcal{N}_{l,\{\mu\}}$  is the normalization constant

$$\mathcal{N}_{l,\{\mu\}}^2 = \frac{1}{2\pi} \times \prod_{j=1}^{D-2} \frac{(\alpha_j + \mu_j)(\mu_j - \mu_{j+1})! [\Gamma(\alpha_j + \mu_{j+1})]^2}{\pi 2^{1-2\alpha_j - 2\mu_{j+1}} \Gamma(2\alpha_j + \mu_j + \mu_{j+1})}, \quad (9)$$

the symbol  $\mathcal{C}_n^{(\lambda)}(t)$  denotes the Gegenbauer polynomial [63, 64] of degree  $n$  and parameter  $\lambda$ , and  $2\alpha_j = D - j - 1$ .

Then, the position probability density of a  $D$ -dimensional hydrogenic state characterized by the hyperquantum numbers  $(n, l, \{\mu\})$  is given by the squared modulus of the position eigenfunction as

$$\begin{aligned} \rho_{n,l,\{\mu\}}(\vec{r}) &= N_{\eta,l}^2 \left[ \frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}} \right] [\mathcal{L}_{\eta-L-1}^{(2L+1)}(\tilde{r})]^2 |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2 \\ &= N_{n,l}^2 \tilde{r}^{2l} e^{-\tilde{r}} [\mathcal{L}_{n-l-1}^{(2l+D-2)}(\tilde{r})]^2 |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2 \\ &\equiv \rho_{n,l}(\tilde{r}) |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2. \end{aligned} \quad (10)$$

Moreover, the Fourier transform of the position eigenfunction  $\Psi_{\eta,l,\{\mu\}}(\vec{r})$  given by (5) provides the eigenfunction of the system in the conjugated momentum space as

$$\tilde{\Psi}_{n,l,\{\mu\}}(\vec{p}) = \mathcal{M}_{n,l}(p) \mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}), \quad (11)$$

where the radial part is

$$\mathcal{M}_{n,l}(p) = K_{n,l} \frac{(\eta\tilde{p})^l}{(1 + \eta^2\tilde{p}^2)^{L+2}} \mathcal{C}_{\eta-L-1}^{(L+1)} \left( \frac{1 - \eta^2\tilde{p}^2}{1 + \eta^2\tilde{p}^2} \right) \quad (12)$$

with  $\tilde{p} = \frac{p}{Z}$  and the normalization constant

$$K_{n,l} = Z^{-\frac{D}{2}} 2^{2L+3} \left[ \frac{(\eta - L - 1)!}{2\pi(\eta + L)!} \right]^{\frac{1}{2}} \Gamma(L + 1) \eta^{\frac{D+1}{2}}. \quad (13)$$

Then, the momentum probability density of the  $D$ -dimensional hydrogenic stationary state with the hyperquantum numbers  $(n, l, \{\mu\})$  is

$$\begin{aligned} \gamma_{n,l,\{\mu\}}(\vec{p}) &= |\tilde{\Psi}_{n,l,\{\mu\}}(\vec{p})|^2 = \mathcal{M}_{n,l}^2(p) |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2 \\ &= K_{n,l}^2 \frac{(\eta\tilde{p})^{2l}}{(1 + \eta^2\tilde{p}^2)^{2L+4}} \left[ \mathcal{C}_{\eta-L-1}^{(L+1)} \left( \frac{1 - \eta^2\tilde{p}^2}{1 + \eta^2\tilde{p}^2} \right) \right]^2 |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2. \end{aligned} \quad (14)$$

### 3. Exact Rényi entropies of the hydrogenic system

In this section we determine the position and momentum Rényi entropies  $R_p[\rho]$  (with natural  $p$  other than unity) for all the discrete stationary states of the  $D$ -dimensional

hydrogenic system in an analytical way. First we note that these entropies can be decomposed into two radial and angular parts in both conjugated spaces. Then, we use a recent procedure [58] based on the Srivastava-Niukkanen method [59, 60, 65] which linearize integer powers of Laguerre and Jacobi polynomials. The involved linearization coefficients are expressed via some multiparametric hypergeometric functions of Lauricella and Srivastava-Daoust types, respectively.

From Eqs. (1), (2) and (10) the Rényi entropies of the  $D$ -dimensional hydrogenic state  $(n, l, \{\mu\})$  in position space can be written as

$$R_q[\rho_{n,l,\{\mu\}}] = R_q[\rho_{n,l}] + R_q[\mathcal{Y}_{l,\{\mu\}}], \quad (15)$$

where  $R_q[\rho_{n,l}]$  denotes the radial part

$$R_q[\rho_{n,l}] = \frac{1}{1-q} \ln \int_0^\infty [\rho_{n,l}]^q r^{D-1} dr, \quad (16)$$

and  $R_q[\mathcal{Y}_{l,\{\mu\}}]$  denotes the angular part

$$R_q[\mathcal{Y}_{l,\{\mu\}}] = \frac{1}{1-q} \ln \Lambda_{l,\{\mu\}}(q), \quad (17)$$

with

$$\Lambda_{l,\{\mu\}}(q) = \int |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^{2q} d\Omega_{D-1}. \quad (18)$$

### 3.1. Radial Rényi entropy in position space

Taking into account Eqs. (10) and (16), the radial Rényi entropy can be written as

$$\begin{aligned} R_q[\rho_{n,l}] &= \frac{1}{1-q} \ln \left[ N_{n,l}^{2q} \int_0^\infty \tilde{r}^{2lq} e^{-q\tilde{r}} [\mathcal{L}_{n-l-1}^{(2l+D-2)}(\tilde{r})]^{2q} r^{D-1} dr \right], \\ &= \frac{1}{1-q} \ln \left[ \lambda^{D(1-q)} \left( \frac{\Gamma(n-l)}{2\eta\Gamma(n+l+D-2)} \right)^q \right] \\ &\quad + \frac{1}{1-q} \ln \int_0^\infty \tilde{r}^{2lq+D-1} e^{-q\tilde{r}} [\mathcal{L}_{n-l-1}^{(2l+D-2)}(\tilde{r})]^{2q} d\tilde{r}. \end{aligned} \quad (19)$$

To evaluate the integral first we perform the change of variable  $x = q\tilde{r}$  to have

$$\begin{aligned} R_q[\rho_{n,l}] &= \frac{1}{1-q} \ln \left[ \lambda^{D(1-q)} \left( \frac{\Gamma(n-l)}{2\eta\Gamma(n+l+D-2)} \right)^q \right] \\ &\quad + \frac{1}{1-q} \ln q^{-D-2lq} \int_0^\infty x^{2lq+D-1} e^{-x} \left[ \mathcal{L}_{n-l-1}^{(2l+D-2)} \left( \frac{x}{q} \right) \right]^{2q} dx, \end{aligned} \quad (20)$$

and then we apply the linearization formula of the  $(2q)$ th-power of the Laguerre polynomial  $L_{n-l-1}^{(2l+D-2)} \left( \frac{x}{q} \right)$  given by

$$y^a \left[ \mathcal{L}_k^{(\alpha)}(ty) \right]^r = \sum_{i=0}^{\infty} c_i(a, r, t, k, \alpha, \gamma) \mathcal{L}_i^{(\gamma)}(y), \quad (21)$$

with  $a > 0, t > 0, \alpha > -1, \gamma > -1$ , the integer  $k \geq 0, i \geq 0$ , and the linearization coefficients

$$c_i(a, r, t, k, \alpha, \gamma) = (\gamma + 1)_a \left( \frac{\Gamma(k + \alpha + 1)}{\Gamma(\alpha + 1)\Gamma(k + 1)} \right)^r \times F_A^{(r+1)} \left( \begin{matrix} \gamma + a + 1; \overbrace{-k, \dots, -k}^r, -i \\ \underbrace{\alpha + 1, \dots, \alpha + 1}_r, \gamma + 1 \quad ; \underbrace{t, \dots, t}_r, 1 \end{matrix} \right), \quad (22)$$

where the Pochhammer symbol  $(z)_a = \frac{\Gamma(z+a)}{\Gamma(z)}$  and the symbol  $F_A^{(s)}(x_1, \dots, x_r)$  denotes the Lauricella function of type A of  $s$  variables and  $2s + 1$  parameters defined as [65]

$$F_A^{(s)} \left( \begin{matrix} a; b_1, \dots, b_s \quad ; x_1, \dots, x_s \\ c_1, \dots, c_s \end{matrix} \right) = \sum_{j_1, \dots, j_s=0}^{\infty} \frac{(a)_{j_1+\dots+j_s} (b_1)_{j_1} \cdots (b_s)_{j_s} x_1^{j_1} \cdots x_s^{j_s}}{(c_1)_{j_1} \cdots (c_s)_{j_s} j_1! \cdots j_s!}. \quad (23)$$

Now, taking  $a = 2lq + D - 1, r = 2q, t = \frac{1}{q}, k = n - l - 1, \alpha = 2l + D - 2$ , inserting (21) in the integral kernel of (20) and using the orthogonalization condition of the Laguerre polynomials [64], after some algebraic manipulations one finds that the final expression of the radial Rényi entropy is given by

$$R_q[\rho_{n,l}] = D \ln \left( \frac{\eta}{2Z} \right) + \frac{q}{1-q} \ln \left( \frac{(\eta - L)_{2L+1}}{2\eta} \right) + \frac{1}{1-q} \ln \mathcal{F}_q(D, \eta, L) + \frac{1}{1-q} \ln \mathcal{A}_q(D, L) \quad (24)$$

where

$$\mathcal{F}_q(D, n, l) \equiv F_A^{(2q)} \left( \begin{matrix} 2lq + D; \overbrace{-n + l + 1, \dots, -n + l + 1}^{2q} \\ \underbrace{2l + D - 1, \dots, 2l + D - 1}_{2q} \quad ; \underbrace{\frac{1}{q}, \dots, \frac{1}{q}}_{2q} \end{matrix} \right), \quad (25)$$

and  $\mathcal{A}_q(D, L) \equiv \frac{\Gamma(D+2lq)}{q^{D+2lq}\Gamma(2L+2)^{2q}}$ . Note that when  $l = n - 1$  the function  $\mathcal{F}_q(D, n, l)$  is equal to unity, so that the third term of the entropy expression (24) vanishes. Moreover, let us highlight that, from Eq. (23), this function defines a finite sum by taking into account the properties of the involved Pochhammer symbols with negative integer arguments.

### 3.2. Angular Rényi entropy

Now, from Eqs. (1), (2), (17), (18) and (8) one has that the angular Rényi entropy has the form

$$R_q[\mathcal{Y}_{l,\{\mu\}}] = \frac{1}{1-q} \ln \int \mathcal{N}_{l,\{\mu\}}^{2q} \prod_{j=1}^{D-2} [\mathcal{C}_{\mu_j - \mu_{j+1}}^{(\alpha_j + \mu_{j+1})}(\cos \theta_j)]^{2q} |\sin \theta_j|^{2q\mu_{j+1}} d\Omega_{D-1} \quad (26)$$

With the change of variable  $t = \cos \theta_j$ , this integral can be rewritten as

$$R_q[\mathcal{Y}_{l,\{\mu\}}] = \frac{1}{1-q} \ln \left( 2\pi \mathcal{N}_{l,\{\mu\}}^{2q} \right) + \frac{1}{1-q} \ln \left[ \prod_{j=1}^{D-2} \mathcal{I}_j(q) \right], \quad (27)$$

where

$$\mathcal{I}_q(D, \mu_j, \mu_{j+1}) = \int_{-1}^1 [\mathcal{C}_{\mu_j - \mu_{j+1}}^{(\alpha_j + \mu_{j+1})}(t)]^{2q} |(1-t^2)|^{q\mu_{j+1} + \alpha_j - \frac{1}{2}} dt. \quad (28)$$

To calculate this integral we use the known relationship between the Gegenbauer and Jacobi polynomials [64],

$$\mathcal{C}_{\kappa}^{(\lambda)}(x) = \frac{\Gamma(\lambda + \frac{1}{2})}{\Gamma(2\lambda)} \frac{\Gamma(\kappa + 2\lambda)}{\Gamma(\kappa + \lambda + \frac{1}{2})} \mathcal{P}_{\kappa}^{(\lambda - \frac{1}{2}, \lambda - \frac{1}{2})}(x) \quad (29)$$

together with the Srivastava-Niukkanen-based linearization formula of the Jacobi polynomials [58]

$$[\mathcal{P}_{\kappa}^{(\alpha, \beta)}(x)]^{2q} = \sum_{i=0}^{\infty} \tilde{c}_i(0, 2q, \kappa, \alpha, \beta, \gamma, \delta) \mathcal{P}_i^{(\gamma, \delta)}(x), \quad (30)$$

with  $\alpha > -1, \beta > -1, \gamma > -1, \delta > -1$  and where the linearization coefficients  $\tilde{c}_i$  are given by

$$\tilde{c}_i(0, 2q, \kappa, \alpha, \beta, \gamma, \delta) = \left( \frac{\Gamma(\kappa + \alpha + 1)}{\Gamma(\alpha + 1)\Gamma(\kappa + 1)} \right)^{2q} \frac{\gamma + \delta + 2i + 1}{\gamma + \delta + i + 1} \times F_{1;1 \dots 1}^{1;2 \dots 2} \left( \begin{matrix} \gamma + 1 : -\kappa, \alpha + \beta + \kappa + 1; \dots; -\kappa, \alpha + \beta + \kappa + 1, -i \\ \gamma + \delta + i + 2 : \alpha + 1; \dots; \alpha + 1, \gamma + 1 \end{matrix} ; 1, \dots, 1 \right) \quad (31)$$

The symbol  $F_{1;1 \dots 1}^{1;2 \dots 2}(x_1, \dots, x_r)$  denotes the  $r$ -variate Srivastava–Daoust function [59] defined as

$$F_{1;1 \dots 1}^{1;2 \dots 2} \left( \begin{matrix} a_0^{(1)} : a_1^{(1)}, a_1^{(2)}; \dots; a_r^{(1)}, a_r^{(2)} \\ \\ b_0^{(1)} : b_1^{(1)}; \dots; b_r^{(1)} \end{matrix} ; x_1, \dots, x_r \right) = \sum_{j_1, \dots, j_r=0}^{\infty} \frac{\binom{a_0^{(1)}}{j_1 + \dots + j_r} \binom{a_1^{(1)}}{j_1} \binom{a_1^{(2)}}{j_1} \dots \binom{a_r^{(1)}}{j_r} \binom{a_r^{(2)}}{j_r} x_1^{j_1} x_2^{j_2} \dots x_r^{j_r}}{\binom{b_0^{(1)}}{j_1 + \dots + j_r} \binom{b_1^{(1)}}{j_1} \binom{b_r^{(1)}}{j_r} j_1! j_2! \dots j_r!}, \quad (32)$$



Then, the orthogonalization relation of the Jacobi polynomials [64]

$$\int_{-1}^1 (1-x)^\alpha (1+x)^\beta P_m^{(\alpha,\beta)}(x) P_n^{(\alpha,\beta)}(x) dx = \frac{2^{\alpha+\beta+1}}{n!} \frac{\Gamma(\alpha+n+1)\Gamma(\beta+n+1)}{(\alpha+\beta+2n+1)\Gamma(\alpha+\beta+n+1)} \delta_{m,n},$$

(for  $\alpha, \beta > -1$ , and where  $\delta_{n,m}$  denotes the Kronecker's delta function) reduces the infinite number of infinite terms of the sum involved in our Gegenbauer linearization to a single one: that for  $i = 0$ . Then, after some algebraic manipulations one obtains that the analytical expression of the angular Rényi entropy is given by

$$\begin{aligned} R_q[\mathcal{Y}_{l,\{\mu\}}] &= \ln(2\pi^{\frac{D}{2}}) + \frac{1}{1-q} \ln \left[ \frac{\Gamma(l + \frac{D}{2})^q \Gamma(qm+1)}{\Gamma(ql + \frac{D}{2}) \Gamma(m+1)^q} \right] \\ &+ \frac{1}{1-q} \sum_{j=1}^{D-2} \ln [\mathcal{B}_q(D, \mu_j, \mu_{j+1}) \mathcal{G}_q(D, \mu_j, \mu_{j+1})] \end{aligned} \quad (33)$$

where

$$\mathcal{B}_q(D, \mu_j, \mu_{j+1}) = \frac{1}{[(\mu_j - \mu_{j+1})!]^q} \frac{(2\alpha_j + 2\mu_{j+1} + 1)_{2(\mu_j - \mu_{j+1})}^q}{(2\alpha_j + \mu_j + \mu_{j+1})_{\mu_j - \mu_{j+1}}^q} \frac{(q\mu_{j+1} + \alpha_j + 1)_{q(\mu_j - \mu_{j+1})}}{(\alpha_j + \mu_{j+1} + 1)_{\mu_j - \mu_{j+1}}^q} \quad (34)$$

and

$$\begin{aligned} \mathcal{G}_q(D, \mu_j, \mu_{j+1}) &= F_{1:1;\dots;1}^{1:2;\dots;2} \left( \begin{array}{c} a_j : b_j, c_j; \dots; b_j, c_j \\ \\ d_j : e_j; \dots; e_j \end{array} ; 1, \dots, 1 \right) \\ &= \sum_{i_1, \dots, i_{2q}=0}^{\mu_j - \mu_{j+1}} \frac{(a_j)_{i_1 + \dots + i_{2q}} (b_j)_{i_1} (c_j)_{i_1} \cdots (b_j)_{i_{2q}} (c_j)_{i_{2q}}}{(d_j)_{i_1 + \dots + i_{2q}} (e_j)_{i_1} \cdots (e_j)_{i_{2q}} i_1! \cdots i_{2q}!} \end{aligned} \quad (35)$$

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

### 3.3. Total Rényi entropy in position space

Finally, from Eqs. (15), (24) and (33) one has that the total Rényi entropy of the  $D$ -dimensional hydrogenic system in position space is given by

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

$$+ \frac{1}{1-q} \sum_{j=1}^{D-2} \ln [\mathcal{B}_q(D, \mu_j, \mu_{j+1}) \mathcal{G}_q(D, \mu_j, \mu_{j+1})] + \ln 2 \quad (36)$$

in terms of the hyperquantum numbers, the nuclear charge and the space dimensionality.

### 3.4. Radial and total Rényi entropy in momentum space

Operating in momentum space in a similar way as done for the position space in subsection 3.1, one has from Eqs. (1), (2) and (14) that the momentum radial Rényi entropy is given by

$$R_q[\gamma_{n,l}] = \frac{1}{1-q} \log \left( \frac{Z^D}{\eta^D} \frac{K_{n,l}^{2q}}{2^{q(L+2)}} \right) + \frac{1}{1-q} \log \int_{-1}^1 (1-y)^{lq + \frac{D}{2} - 1} (1+y)^{D(q-\frac{1}{2}) + q(l+1) - 1} \mathcal{C}_{n-l-1}^{(L+1)}(y)^{2q} dy$$

Again the use of the relation (29) and the Srivastava-Niukkanen-based linearization formula (30) of the Jacobi polynomials has led us to find the following expression of the radial part of the Rényi entropy in momentum space:

$$R_q[\gamma_{n,l}] = D \log \frac{Z}{\eta} + \frac{q}{1-q} \log [2\eta(\eta-L)_{2L+1}] + \frac{1}{1-q} \log \overline{\mathcal{F}}_q(D, \eta, L) + \frac{1}{1-q} \log \overline{\mathcal{A}}_q(D, L) \quad (37)$$

where

$$\overline{\mathcal{F}}_q(D, \eta, L) \equiv F_{1:1; \dots; 1}^{1:2; \dots; 2} \left( \begin{matrix} a : b, c; \dots; b, c \\ \\ d : e; \dots; e \end{matrix} ; 1, \dots, 1 \right) = \sum_{i_1, \dots, i_{2q}=0}^{n-l-1} \frac{(a)_{i_1+\dots+i_{2q}} (b)_{i_1} (c)_{i_1} \dots (b)_{i_{2q}} (c)_{i_{2q}}}{(d)_{i_1+\dots+i_{2q}} (e)_{i_1} \dots (e)_{i_{2q}} i_1! \dots i_{2q}!} \quad (38)$$

with  $a = (L + \frac{3}{2})q + \frac{D}{2}(1-q)$ ,  $b = -(\eta - L - 1)$ ,  $c = \eta + L + 1$ ,  $d = q(2L + 4)$ ,  $e = L + \frac{3}{2}$  and

$$\overline{\mathcal{A}}_q(D, L) \equiv 2^{2q-1} \frac{\Gamma(\frac{D}{2} + ql) \Gamma(-\frac{D}{2} + q(D + l + 1))}{\Gamma(\frac{D}{2} + l)^{2q} \Gamma(q(D + 2l + 1))} \quad (39)$$

Note that, when  $l = n - 1$  the function  $\mathcal{F}_q(D, \eta, L) = 1$ .

Finally, since the angular part of the momentum Rényi entropy is the same as in position space, one obtains from Eqs. (38) and (33) that the total Rényi entropy in

momentum space  $R_q[\gamma_{n,L,\{\mu_j\}}] = R_q[\gamma_{n,l}] + R_q[\mathcal{Y}_{l,\{\mu\}}]$  has the following expression

$$\begin{aligned} R_q[\gamma_{n,l,\{\mu\}}] &= D \log \left( \frac{\pi^{\frac{1}{2}} Z}{\eta} \right) + \frac{q}{1-q} \log [2\eta (\eta - L)_{2L+1}] \\ &+ \frac{1}{1-q} \log \left[ \overline{\mathcal{F}}_q(D, \eta, L) \overline{\mathcal{A}}_q(D, L) \frac{\Gamma(l + \frac{D}{2})^q \Gamma(qm + 1)}{\Gamma(ql + \frac{D}{2}) \Gamma(m + 1)^q} \right] \\ &+ \frac{1}{1-q} \sum_{j=1}^{D-2} \log [\mathcal{B}_q(D, \mu_j, \mu_{j+1}) \mathcal{G}_q(D, \mu_j, \mu_{j+1})] + \log 2 \end{aligned} \quad (40)$$

in terms of the hyperquantum numbers, the nuclear charge and the space dimensionality.

### 3.5. Rényi entropies for the quasi-spherical $ns$ states

To illustrate the applicability of the previous position and momentum Rényi entropies, we calculate them for a relevant class of specific states of the  $D$ -dimensional hydrogenic system which include the ground state: the quasi-spherical  $ns$  states, which are characterized by the angular hyperquantum numbers  $\mu_1 = \mu_2 \dots = \mu_{D-1} = l$ . First, since  $l = n - 1$ , the Lauricella function of Eq. (24) is equal to unity. Then, we find the values

$$R_q[\rho_{n,n-1}] = D \log \frac{\eta}{2Z} - \frac{q}{1-q} \log [\Gamma(2\eta + 1)] + \frac{1}{1-q} \log \left( \frac{\Gamma(D + 2nq - 2q)}{q^{D+2nq-2q}} \right) \quad (41)$$

for the radial Rényi entropy of the  $ns$  states in position space, and

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

for the corresponding one of the ground state ( $n=1$ ). In addition, we have found the values

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

and

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

for the angular Rényi entropy of the  $ns$  states and the ground state, respectively. Similar operations in the momentum space have allowed us to have the values

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

and

$$R_q[\gamma_{1,0}] = D \log \left[ \frac{2Z}{D-1} \right] + \frac{q}{1-q} \log [4\Gamma(D)]$$

$$+ \frac{1}{1-q} \log \left[ \frac{\Gamma\left(\frac{D}{2}\right)^{1-2q} \Gamma\left(D\left(q - \frac{1}{2}\right) + q\right)}{2\Gamma(Dq + q)} \right]$$

for for the radial Rényi entropy of the  $ns$  states and the ground state in momentum space, respectively.

Finally, we gather in Tables 1 and 2 the exact values of the position and momentum Rényi entropies  $R_2[\rho_{n,l,m}]$  and  $R_2[\gamma_{n,l,m}]$ , respectively, of various quasi-circular circular states of the three-dimensional hydrogen atom.

$R_2[\rho_{n,l,m}]$	$n = 1$	$n = 2$	$n = 3$
$l = 0, m = 0$	$\log(8\pi)$	$\log\left(\frac{2048\pi}{5}\right)$	$\log\left(\frac{84934656\pi}{5}\right)$
$l = 1, m = 0$	-	$\log\left(\frac{2048\pi}{9}\right)$	$\log\left(\frac{27648\pi}{11}\right)$
$l = 1, m = 1$	-	$\log\left(\frac{1024\pi}{3}\right)$	$\log\left(\frac{41472\pi}{11}\right)$
$l = 2, m = 0$	-	-	$\log\left(\frac{9216\pi}{5}\right)$
$l = 2, m = 1$	-	-	$\log\left(\frac{13824\pi}{5}\right)$
$l = 2, m = 2$	-	-	$\log\left(\frac{13824\pi}{5}\right)$

**Table 1.** Exact values of the total position Rényi entropy  $R_2[\rho_{n,l,m}]$  for various quasi-circular states of the three-dimensional hydrogen atom.

$R_2[\gamma_{n,l,m}]$	$n = 1$	$n = 2$	$n = 3$
$l = 0, m = 0$	$\log\left(\frac{16\pi^2}{33}\right)$	$\log\left(\frac{2\pi^2}{151}\right)$	$\log\left(\frac{16\pi^2}{7533}\right)$
$l = 1, m = 0$	-	$\log\left(\frac{2\pi^2}{39}\right)$	$\log\left(\frac{160\pi^2}{36207}\right)$
$l = 1, m = 1$	-	$\log\left(\frac{\pi^2}{13}\right)$	$\log\left(\frac{80\pi^2}{12069}\right)$
$l = 2, m = 0$	-	-	$\log\left(\frac{1120\pi^2}{78489}\right)$
$l = 2, m = 1$	-	-	$\log\left(\frac{560\pi^2}{26163}\right)$
$l = 2, m = 2$	-	-	$\log\left(\frac{560\pi^2}{26163}\right)$

**Table 2.** Exact values of the total momentum Rényi entropy  $R_2[\gamma_{n,l,m}]$  for various quasi-circular states of the three-dimensional hydrogen atom.

#### 4. Position-momentum Rényi-entropy sum

Here we give the joint position-momentum Rényi uncertainty sum for all the discrete stationary states of the  $D$ -dimensional hydrogenic system from Eqs. (36) and (40). We obtain

$$\begin{aligned}
R_q[\rho_{n,l,\{\mu\}}] + R_p[\gamma_{n,l,\{\mu\}}] &= D \log \left( \frac{\pi}{2} \right) + \frac{2q}{q-1} \log [2\eta] \\
&+ \log \left[ \mathcal{F}_q(D, \eta, L)^{\frac{1}{1-q}} \overline{\mathcal{F}}_p(D, \eta, L)^{\frac{1}{1-p}} \mathcal{A}_q(D, L)^{\frac{1}{1-q}} \overline{\mathcal{A}}_p(D, L)^{\frac{1}{1-p}} \right] \\
&+ \log \left[ \left( \frac{\Gamma(qm+1)}{\Gamma(ql + \frac{D}{2})} \right)^{\frac{1}{1-q}} \left( \frac{\Gamma(pm+1)}{\Gamma(pl + \frac{D}{2})} \right)^{\frac{1}{1-p}} \right] \\
&+ \sum_{j=1}^{D-2} \log \left[ (q\mu_{j+1} + \alpha_j + 1)_{q(\mu_{j+1}-\mu_j)}^{\frac{1}{1-q}} (p\mu_{j+1} + \alpha_j + 1)_{p(\mu_{j+1}-\mu_j)}^{\frac{1}{1-p}} \right] \\
&+ \sum_{j=1}^{D-2} \log \left[ (\mathcal{G}_q(D, \mu_j, \mu_{j+1}))^{\frac{1}{1-q}} (\mathcal{G}_p(D, \mu_j, \mu_{j+1}))^{\frac{1}{1-p}} \right] + \log 4 \quad (42)
\end{aligned}$$

with  $\frac{1}{p} + \frac{1}{q} = 2\ddagger$ . When the spatial dimension is  $D = 3$  this expression boils down to

$$\begin{aligned}
R_q[\rho_{n,l,m}] + R_p[\gamma_{n,l,\{\mu_j\}}] &= 3 \log \left( \frac{\pi}{2} \right) + \frac{2q}{q-1} \log [2n] \\
&+ \log \left[ \mathcal{F}_q(3, n, l)^{\frac{1}{1-q}} \overline{\mathcal{F}}_p(3, n, l)^{\frac{1}{1-p}} \mathcal{A}_q(3, l)^{\frac{1}{1-q}} \overline{\mathcal{A}}_p(3, l)^{\frac{1}{1-p}} \right] \\
&+ \log \left[ (\mathcal{G}_q(3, l, m))^{\frac{1}{1-q}} (\mathcal{G}_p(3, l, m))^{\frac{1}{1-p}} \right] \\
&+ \log \left[ 4 \left( \frac{\Gamma(qm+1)}{\Gamma(qm + \frac{3}{2})} \right)^{\frac{1}{1-q}} \left( \frac{\Gamma(pm+1)}{\Gamma(pm + \frac{3}{2})} \right)^{\frac{1}{1-p}} \right] \quad (43)
\end{aligned}$$

Finally and most interesting, the expression (42) in the limit  $D \rightarrow \infty$  becomes

$$R_q[\rho_{\eta,L,\{\mu_j\}}] + R_p[\gamma_{\eta,L,\{\mu_j\}}] \sim D \log \left( 2\pi(2q)^{\frac{1}{2-2q}} (2p)^{\frac{1}{2-2p}} \right), \quad (44)$$

which is the saturation value of the Rényi-entropy-based uncertainty relation found independently by Bialynicki-Birula [66] and Zozor-Portesi-Vignat [67, 68].

$$R_q[\rho] + R_p[\gamma] \geq D \log \left( 2\pi(2q)^{\frac{1}{2-2q}} (2p)^{\frac{1}{2-2p}} \right), \quad \frac{1}{p} + \frac{1}{q} = 2. \quad (45)$$

This fact is not only a partial checking of our results but also it is in accordance with similar findings obtained in a very different way.

‡ In fact, this is only valid provided the functions  $\mathcal{F}_q, \overline{\mathcal{F}}_q$  and  $\mathcal{G}_q$  exist for any  $p, q \in \mathbb{R}$ .

## 5. Conclusions

In this work we have explicitly calculated the total position  $R_q[\rho_{n,l,\{\mu\}}]$  and momentum  $R_q[\gamma_{n,l,\{\mu\}}]$  Rényi entropies (with integer  $q$  greater than 1) for all the quantum-mechanically allowed hydrogenic states in terms of the Rényi parameter  $q$ , the spatial dimension  $D$ , the nuclear charge  $Z$  as well as the hyperquantum numbers,  $(n, l, \{\mu\})$ , which characterize the corresponding wavefunction of the states. To do that we have used a recent methodology which allows to determine the involved integral functionals by taking into account the linearization formula and orthogonality conditions of the Laguerre and Jacobi polynomials; the latter ones are closely connected to the Gegenbauer polynomials which control the angular part of the wavefunctions in both conjugated spaces as well as the radial wavefunction in momentum space. The final expressions for the Rényi entropies in position and momentum spaces are expressed in a compact way by use of a multivariate hypergeometric function of Lauricella and Srivastava-Daoust types evaluated at  $1/q$  and unity, respectively; indeed, note that all sums to be evaluated are finite. Finally, it remains as an open problem the extension of this result to the limiting case  $q \rightarrow 1$ , which corresponds to the Shannon entropy, and the Rényi entropies for any real value of the parameter  $q$ . The latter requires a completely different approach, still unknown to the best of our knowledge.

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## Chapter 3

# Rényi and Shannon entropies of harmonic systems

The study of the harmonic (oscillator-like) systems has been central in the development of classical and quantum mechanics. This is because when a particle is close to its equilibrium position, the potential which governs the dynamics can be approximated by the harmonic potential. The multidimensional harmonic system (i.e., a particle moving under the action of a quadratic quantum-mechanical potential) [56] is, together with the hydrogenic system, the main prototype of the physics of multidimensional quantum systems. This model have long been regarded as an important laboratory toolbox in numerous scientific fields from quantum chemistry to quantum information, mainly because it is a completely integrable analogue of many body systems due to their remarkable analytic properties. Indeed, the multidimensional harmonic system has been shown to be very effective in the description of e.g. quantum dots, ultracold gases in harmonic traps, fractional quantum Hall effect and quark confinement [156–165]. Despite this increasing interest from both theoretical and applied standpoints, there does not exit a deep knowledge about the Heisenberg and entropy-like uncertainty measures of the  $D$ -dimensional harmonic oscillator, although a number of related works have been carried out [34, 35, 37, 42, 117, 166–182].

These measures, which quantify the spreading properties of the harmonic probability density, are respectively characterized by the radial expectation values and the Rényi and Shannon entropies of the corresponding quantum probability density of the system in position and momentum spaces.

The goal of the present Chapter is to determine the Heisenberg-like and entropic uncertainty measures (as given by the radial expectation values and the Rényi entropies, respectively) of the multidimensional harmonic system for the extreme states of Rydberg [64] and pseudo-classical states [65] and for general stationary states [66] in the two conjugated spaces of position and momentum types.

The chapter is composed by three sections. Briefly, the main results of each section are the following:

- 3.1 The angular and radial contributions to the position and momentum entropic uncertainty measures for the highly-excited (Rydberg) states of the multidimensional harmonic system are analytically expressed in terms of the hyperquantum numbers which characterize the corresponding quantum states and, for the radial part, the oscillator strength [64].
- 3.2 The leading term of the Heisenberg-like and entropy-like uncertainty measures for the high-dimensional states of the multidimensional harmonic system is obtained in a closed form. The associated multidimensional position-momentum uncertainty relations are discussed, showing that they saturate the corresponding general ones [65].
- 3.3 The exact values of the Rényi uncertainty measures of the  $D$ -dimensional harmonic system are determined for all ground and excited quantum states directly in terms of  $D$ , the potential strength and the hyperquantum numbers. They can be expressed in a compact way by use of a generalized hypergeometric Lauricella function of type A [66].

### 3.1 Rydberg states

In this section we explicitly determine the Shannon, Rényi and Tsallis information-theoretic measures of the highly excited (i.e., Rydberg) quantum states of the multidimensional harmonic system in terms of the basic parameters which characterize the system; that is, the dimensionality  $D$ , the hyperquantum numbers and the oscillator strength. This has been possible through the use of the novel mathematical technique developed by Aptekarev et al. [122] which has been briefly described in the Section 1.2, and the use of the linearization and expansion methods for orthogonal polynomials described in Section 1.3.

This aim has required to carry out the following tasks:

- To obtain two equivalent analytical expressions for the angular contribution to the Rényi entropy of the probability density which characterizes the quantum states of any central potential. They have been developed by means of the polynomial linearization and expansion methodologies described in Theorems 1.6 and Lemma 1.8 of Section 1.3, respectively.
- To determine the leading term of the radial contribution to the Rényi entropy for the Rydberg states of the  $D$ -dimensional harmonic system, what is specially

remarkable because it is a serious problem even numerically. This has been done by Theorem 1.1 of Aptekarev et al. [122] briefly described in the Sec. 1.2

- To illustrate the applicability of the previous findings by applying them to some specific Rydberg harmonic states of  $ns$  and  $np$  types.
- To calculate and discuss the position-momentum Rényi and Shannon uncertainty sums for a large class of Rydberg harmonic states which include the ground state.

These results have been published in the article [64] with coordinates: Dehesa J. S., Toranzo I. V. and **Puertas-Centeno D.** *Entropic measures of Rydberg-like harmonic states*. International Journal of Quantum Chemistry, 117:48-56, 2017, which is attached below.

# Entropic measures of Rydberg-like harmonic states

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The Shannon entropy, the disequilibrium and their generalizations (Rényi and Tsallis entropies) of the three-dimensional single-particle systems in a spherically-symmetric potential  $V(r)$  can be decomposed into angular and radial parts. The radial part depends on the analytical form of the potential, but the angular part does not. In this paper we first calculate the angular entropy of any central potential by means of two analytical procedures. Then, we explicitly find the dominant term of the radial entropy for the highly energetic (i.e., Rydberg) stationary states of the oscillator-like systems. The angular and radial contributions to these entropic measures are analytically expressed in terms of the quantum numbers which characterize the corresponding quantum states and, for the radial part, the oscillator strength. In the latter case we use some recent powerful results of the information theory of the Laguerre polynomials and spherical harmonics which control the oscillator-like wavefunctions.

Keywords: Entropic measures of Rydberg oscillator states, Information theory of the harmonic oscillator, Angular entropies of any central potential, Rényi and Tsallis entropies of the harmonic oscillator, Shannon entropy of the harmonic oscillator.

## I. INTRODUCTION

The classical and quantum entropies of the many-particle systems, which are functionals of the one-particle quantum-mechanical probability density, do not only quantify the spatial delocalization of this density in various complementary ways and describe a great deal of physical and chemical properties of the systems but also they are the fundamental variables of the information theory of quantum systems which is at the basis of the modern Quantum Information. The computational determination of these quantities is a formidable task (not yet solved, except possibly for the ground and a few lowest-lying energetic states), even for the small bunch of elementary quantum potentials which are used to approximate the mean-field potential of the physical systems [1–5].

The harmonic oscillator is both a pervasive concept in science and technology and a fundamental building block in our system of knowledge of the physical universe [6, 7]. Indeed it has been applied from the physics of quarks to quantum cosmology. The harmonic oscillator is, together with the Coulomb potential, the most relevant quantum-mechanical potential for the description of the structure and dynamics of natural systems. It has played *per se* a crucial role in the development of quantum physics since its birth [8], mainly because the wave functions of its quantum-mechanically allowed oscillator-like states can be explicitly expressed in terms of special functions of mathematical physics (namely, the Laguerre polynomials and spherical harmonics). Moreover, it has provided an approximate model for the physically-correct quantum-mechanical potentials of many-particle systems what is very useful for the the interpretation and quantitative estimation of numerous microscopic and macroscopic properties of natural systems. Indeed, it seems that this paradigmatic oscillator-like formalisation relies on the so-called *mean-field* approximation: each particle harmonically interacts with all others in the system, regardless of their reciprocal distance. Moreover, the solutions of the wave equations of complex physical systems within this approximation are very valuable, referencial tools for checking and improving complicated numerical methods used to study such systems.

Let us just highlight that the oscillator wave functions saturate the most important mathematical realizations of the quantum uncertainty principle such as the Heisenberg-like [9, 10] uncertainty relations, which are based on the variance and/or higher-order moments, and the entropic uncertainty relations based on the Shannon entropy [11, 12], the Rényi entropy [13, 14] or the Fisher information [9, 15]. Furthermore, they have been used in numerous scientific fields ranging from quantum many-body physics [16–24], heat transport [25], quantum entanglement [26, 27],

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Kepler systems [28], quantum dots [18, 29, 30] and cold atomic gases [31, 32] to fractional and quantum statistics [33, 34] and black-holes thermodynamics [35, 36]. However, the information-theoretic properties of the three (or higher)-dimensional harmonic oscillator are not yet settled down in spite of numerous efforts (see e.g., [2, 3, 37]), mainly because of the yet incomplete knowledge of the information theory of orthogonal polynomials and spherical harmonics [38–41].

In this work we first realize that the information entropies (Shannon, Rényi and Tsallis) of the three-dimensional single-particle systems in a spherically-symmetric potential  $V(r)$  can be decomposed into two angular and radial parts. The radial part depends on the analytical form of the potential, but the angular part does not. Then, we determine both the angular contribution to these entropies for all the quantum-mechanically allowed states of the central potential  $V(r)$  and the radial entropy of the highly-energetic (i.e., Rydberg) states of the (three-dimensional) harmonic oscillator in an analytical way. The latter is done by using some recent powerful results of the information theory of Laguerre and Gegenbauer polynomials [4, 42–44] (see also [45, 46]).

The structure of the work is the following. In section II we first describe the information entropies of an arbitrary probability density to be used; later we apply them to a single-particle system subject to a central potential  $V(r)$ , showing that they can be decomposed into radial and angular parts, with emphasis on the Rényi entropy from which all the remaining entropies can be analytically obtained. Then, we begin to calculate the information entropies of the oscillator-like states by collecting all the necessary data, particularly the quantum probability density which define these states. In section III we tackle the computation of the angular part of the Rényi entropy for all quantum states of any central potential by means of two different analytical procedures. In Section IV we first calculate the dominant term of the radial part of the Rényi and Shannon entropies of the highly-energetic (i.e., Rydberg) oscillator-like states. Then, the total Rényi and Shannon entropies can be analytically obtained in a straightforward way, what is illustrated for some specific Rydberg oscillator-like states. In Section V we illustrate that the information entropies of the low-energy states can be calculated in a analytical, much simpler way; and, moreover, we show that the position and momentum values of the Shannon and Rényi entropies found for the states lying at the two extreme regions of the spectrum verify the position-momentum Shannon-entropy-based [11, 12] and Rényi-entropy-based [13, 14] uncertainty relations, respectively. Finally, some conclusions are given.

## II. INFORMATION ENTROPIES OF QUANTUM STATES

In this section we define the basic information entropies of a probability density  $\rho(\vec{r})$ ; namely, the Rényi and Tsallis entropies and their instances, the Shannon entropy and the disequilibrium. Then, we study these quantities for the quantum-mechanically allowed states of a physical system with a spherically-symmetric potential  $V(r)$ , pointing out that they can be decomposed into two angular and radial parts. Finally, we explicitly apply them to the oscillator-like states. Atomic units are used throughout the paper.

The  $p$ th-order Rényi entropy  $R_p[\rho]$  of the density  $\rho(\vec{r})$  is defined [47] as

$$R_p[\rho] = \frac{1}{1-p} \ln \int_{\mathbb{R}^3} [\rho(\vec{r})]^p d\vec{r}; \quad 0 < p < \infty, p \neq 1, \quad (1)$$

and the Tsallis entropy [48], given by  $T_p[\rho] = \frac{1}{p-1} (1 - \int_{\mathbb{R}^3} [\rho(\vec{r})]^p d\vec{r})$ , can be obtained from the Rényi one by means of the expression

$$T_p[\rho] = \frac{1}{1-p} \left( e^{(1-p)R_p[\rho]} - 1 \right). \quad (2)$$

These two sets of entropies globally quantify different facets of the spreading of the probability cloud all over the spatial volume where the density function  $\rho(\vec{r})$  is defined. All the members of each set completely characterize the density under certain conditions [49, 50]. Some of them are very relevant *per se* such as e.g., the Shannon entropy (which measures the total extent of the density),  $S[\rho] := - \int \rho(\vec{r}) \ln \rho(\vec{r}) d\vec{r} = \lim_{p \rightarrow 1} R_p[\rho] = \lim_{p \rightarrow 1} T_p[\rho]$ , and the disequilibrium (which quantifies the separation of the density with respect to equiprobability),  $\langle \rho \rangle = \exp(-R_2[\rho]) = 1 - T_2[\rho]$ . See [49–58] for further knowledge of these quantities. Let us just mention that the Rényi entropies and their associated uncertainty relations have been widely used to investigate numerous quantum-mechanical properties and phenomena of physical systems and processes [13, 56–58], the pattern formation and Brown processes [59, 60], fractality and chaotic systems [61, 62], quantum phase transition [63] and the quantum-classical correspondence [64] and quantum

entanglement [65, 66].

The probability density  $\rho(\vec{r})$  of a single-particle system subject to the central potential  $V(r)$  is given by the squared modulus of the position eigenfunction  $\Psi(\vec{r})$ , which satisfies the Schrödinger equation

$$\left(-\frac{1}{2}\vec{\nabla}^2 - V(r)\right)\Psi(\vec{r}) = E\Psi(\vec{r}), \quad (3)$$

where the position vector  $\vec{r} = (x_1, x_2, x_3)$  in polar spherical units is given as  $(r, \theta, \phi) \equiv (r, \Omega)$ ,  $\Omega \in S^2$ , where  $r \equiv |\vec{r}| = \sqrt{\sum_{i=1}^3 x_i^2} \in [0; +\infty)$  and with  $\theta \in [0; \pi)$ ,  $\phi \in [0; 2\pi)$ . It is well known that the eigenfunction factorizes as  $\Psi_{n,l,m}(\vec{r}) = \mathcal{R}_{n,l}(r) Y_{l,m}(\Omega)$ , where the radial part  $\mathcal{R}_{n,l}(r)$  depends on the analytical form of the potential and the angular part  $Y_{l,m}(\Omega)$  is given by the spherical harmonics defined [67] by

$$Y_{l,m}(\theta, \varphi) = A_{l,m} e^{im\varphi} (\sin\theta)^m C_{l-m}^{(m+\frac{1}{2})}(\cos\theta) \quad (4)$$

with the normalization constant is

$$A_{l,m} = \sqrt{\frac{(l+\frac{1}{2})(l-m)! [\Gamma(m+\frac{1}{2})]^2}{2^{1-2m} \pi^2 (l+m)!}},$$

and the symbol  $C_n^{(\lambda)}(t)$  denotes the Gegenbauer polynomial of degree  $n$  and parameter  $\lambda$ . Then, the probability density of the quantum stationary state  $(n, l, m)$  is given by

$$\rho_{n,l,m}(\vec{r}) = \rho_{n,l}(r) |Y_{l,m}(\Omega)|^2, \quad (5)$$

where the radial part is the univariate function  $\rho_{n,l}(r) = [\mathcal{R}_{n,l}(r)]^2$ . Now we can compute the information entropies of this density. From Eqs. (1) and (5) we obtain that the Rényi entropies of the quantum state  $(n, l, m)$  can be expressed as

$$R_p[\rho_{n,l,m}] = R_p[\rho_{n,l}] + R_p[Y_{l,m}], \quad (6)$$

where  $R_p[\rho_{n,l}]$  denotes the radial part

$$R_p[\rho_{n,l}] = \frac{1}{1-p} \ln \int_0^\infty [\rho_{n,l}]^p r^2 dr, \quad (7)$$

and  $R_p[Y_{l,m}]$  denotes the angular part

$$R_p[Y_{l,m}] = \frac{1}{1-p} \ln \Lambda_{l,m}. \quad (8)$$

with

$$\Lambda_{l,m} = \int_{S^2} |Y_{l,m}(\theta, \phi)|^{2p} d\Omega. \quad (9)$$

For  $p = 1$  and  $2$  we obtain similar expressions for the disequilibrium and Shannon entropy, respectively. In particular, the Shannon entropy of the quantum state  $(n, l, m)$  of any central potential is decomposed as

$$S[\rho_{n,l,m}] = S[\rho_{n,l}] + S[Y_{l,m}], \quad (10)$$

where the radial and angular parts are given by

$$S[\rho_{n,l}] = \lim_{p \rightarrow 1} R_p[\rho_{n,l}], \quad (11)$$

and

$$S[Y_{l,m}] = \lim_{p \rightarrow 1} R_p[Y_{l,m}], \quad (12)$$

respectively. Note that, contrary to the radial parts, the angular parts  $R_p[Y_{l,m}]$  and  $S[Y_{l,m}]$  do not depend on the analytical form of the potential  $V(r)$ . Surprisingly, these angular Rényi and Shannon entropies have never been

calculated up to now. We will do it in the next section III.

To go forward into the radial Rényi entropy  $R_p[\rho_{n,l}]$ , we will take into account the oscillator potential  $V(r) = \frac{1}{2}\lambda^2 r^2$  whose Schrödinger equation (3) is known (see e.g., [37, 68]) to be exactly solved, so that the energetic eigenvalues are

$$E_{n,l} = \lambda \left( 2n + l + \frac{3}{2} \right), \quad (13)$$

and the corresponding eigenfunctions are expressed as

$$\begin{aligned} \Psi_{n,l,m}(\vec{r}) &= \left[ \frac{2n!\lambda^{l+\frac{3}{2}}}{\Gamma(n+l+\frac{3}{2})} \right]^{\frac{1}{2}} r^l e^{-\frac{\lambda r^2}{2}} L_n^{(l+1/2)}(\lambda r^2) \\ &\times Y_{l,m}(\Omega), \end{aligned} \quad (14)$$

with  $(n = 0, 1, 2, \dots; l = 0, 1, 2, \dots; m = -l, -l+1, \dots, +l)$ , and  $L_n^{(\alpha)}(t)$  denotes [67] the Laguerre polynomial of parameter  $\alpha$  and degree  $n$ .

Then, the position probability density of the isotropic harmonic oscillator has the form (5) where the radial part is given by

$$\begin{aligned} \rho_{n,l}(r) &= \frac{2n!\lambda^{l+\frac{3}{2}}}{\Gamma(n+l+\frac{3}{2})} r^{2l} e^{-\lambda r^2} \left[ L_n^{(l+1/2)}(\lambda r^2) \right]^2 \\ &= \frac{2n!\lambda^{\frac{3}{2}}}{\Gamma(n+l+\frac{3}{2})} x^{\frac{1}{2}} \omega_{l+\frac{1}{2}}(x) \left[ L_n^{(l+1/2)}(x) \right]^2 \\ &= 2\lambda^{\frac{3}{2}} \frac{\omega_{l+\frac{1}{2}}(x)}{x^{-1/2}} \left[ \widehat{L}_n^{(l+1/2)}(x) \right]^2 \end{aligned} \quad (15)$$

where  $x = \lambda r^2$  and

$$\omega_\alpha(x) = x^\alpha e^{-x}, \quad \alpha = l + \frac{1}{2}, \quad (16)$$

is the weight function of the orthogonal and orthonormal Laguerre polynomials of degree  $n$  and parameter  $\alpha$ , here denoted by  $L_n^{(\alpha)}(x)$  and  $\widehat{L}_n^{(\alpha)}(x)$ , respectively. Moreover, it is known [37] that the probability density in momentum space (i.e., the squared modulus of the Fourier transform of the position eigenfunction) is given by  $\gamma(\vec{p}) = \frac{1}{\lambda^3} \rho\left(\frac{\vec{p}}{\lambda}\right)$ . So, the position and momentum information entropies of the oscillator-like states have a formal expression of similar type.

Later on, in Section IV, we will determine in an analytical way the radial Rényi and Shannon entropies not for all quantum oscillator-like states (what is an open problem) but *only* for all highly energetic (i.e., Rydberg) oscillator-like states. The Rydberg case is even a serious computational task because it involves the numerical evaluation of the Rényi and Shannon functionals of Laguerre polynomials  $L_n(x)$  with a high and very high degree  $n$ . Indeed, a naive use of quadratures to tackle this problem is not convenient: since all the zeros of  $L_n(x)$  belong to the interval of orthogonality, the increasing number of integrable singularities spoil any attempt to achieve reasonable accuracy even for rather small  $n$  [69]. Finally, let us advance here that the information entropies for the low-energy states can be easily obtained because then the corresponding Laguerre polynomials have low degrees so that the associated entropic integrals can be solved in an analytically simple manner, as it is illustrated in Section V.

### III. ANGULAR ENTROPIES OF QUANTUM STATES OF ANY CENTRAL POTENTIAL

In this section we describe two qualitatively different analytical procedures for the evaluation of the angular Rényi entropy  $R_p[Y_{l,m}]$ , given by (8), of any quantum state of an arbitrary central potential. Then, the corresponding

angular Shannon entropies follow in the limit  $p \rightarrow 1$ . We start with Eqs. (9) and (4) to obtain the angular functional

$$\Lambda_{l,m} = \int_{\mathbb{S}^2} |Y_{l,m}(\theta, \phi)|^{2p} d\Omega \quad (17)$$

$$\begin{aligned} &= 2\pi [A_{l,m}]^{2p} \int_0^\pi |C_{l-m}^{(m+1/2)}(\cos \theta)|^{2p} (\sin \theta)^{2pm+1} d\theta. \\ &= 2\pi [A_{l,m}]^{2p} \int_{-1}^1 |C_{l-m}^{(m+1/2)}(t)|^{2p} (1-t^2)^{mp} dt \end{aligned} \quad (18)$$

To compute (18) we propose the two following methods. One based on the linearization technique of Srivastava [42, 45] and another one based on the power expansion via the Bell polynomials [44, 46].

### A. Linearization-based method

The functional of Gegenbauer polynomials of (18) can be solved by means of the linearization formula of Srivastava [42, 45] for the natural powers of Jacobi polynomials. Indeed, since the Gegenbauer polynomials are particular instances of Jacobi polynomials as indicated by

$$C_n^{(\lambda)}(t) = \frac{(2\lambda)_n}{(\lambda + \frac{1}{2})_n} P_n^{(\lambda - \frac{1}{2}, \lambda - \frac{1}{2})}(t), \quad (19)$$

where  $\lambda = m + 1/2$  and  $n = l - m$ . we have that the angular functional  $\Lambda_{l,m}$  can be rewritten as

$$\Lambda_{l,m} = A'_{l,m} \int_{-1}^1 |P_{l-m}^{(m,m)}(t)|^{2p} (1-t)^{mp} (1+t)^{mp} dt, \quad (20)$$

where

$$A'_{l,m} = \frac{2^{2(m-1)p+1} (2l+1)^p}{\pi^{2p-1}} \left[ \frac{\Gamma(m + \frac{1}{2})^2 (l-m)! (m!)^2 (l+m)!}{(l!)^2 [(2m)!]^2} \right]^p \quad (21)$$

Then, the Srivastava linearization formula appropriately modified for our purposes gives [42]

$$\left[ P_{l-m}^{(m,m)}(t) \right]^{2p} = \sum_{i=0}^{\infty} \tilde{c}_i(p, l, m) P_i^{(pm, pm)}(t), \quad (22)$$

(which holds for positive integer and half-integer values of the parameter  $p$ ), where the coefficients  $\tilde{c}_i(p, l, m)$  (or equivalently  $\tilde{c}_i(0, 2p, l - m, m, m, pm, pm)$  in the notation of [42]) have the expression

$$\begin{aligned} \tilde{c}_i(p, l, m) &= \binom{l}{l-m}^{2p} \frac{2mp + 2i + 1}{2mp + i + 1} \sum_{j_1, \dots, j_{2p}=0}^{l-m} \sum_{j_{2p+1}=0}^i \frac{(mp+1)_{j_1+\dots+j_{2p}+j_{2p+1}}}{(2mp+i+2)_{j_1+\dots+j_{2p}}} \\ &\times \frac{(m-l)_{j_1} (l+m+1)_{j_1} \cdots (m-l)_{j_{2p}} (l+m+1)_{j_{2p}} (-i)_{j_{2p+1}}}{(m+1)_{j_1} \cdots (m+1)_{j_{2p}} (pm+1)_{j_{2p+1}} j_1! \cdots j_{2p}! j_{2p+1}!}. \end{aligned} \quad (23)$$

Substituting (22) into (20) and using the orthogonality property of the Jacobi polynomials

$$\int_{-1}^1 (1-t)^a (1+t)^b P_n^{(a,b)}(t) P_m^{(a,b)}(t) dt = \frac{2^{a+b+1} \Gamma(a+n+1) \Gamma(b+n+1)}{n! (a+b+2n+1) \Gamma(a+b+n+1)} \delta_{m,n}, \quad (24)$$

we obtain the following expression for the angular functional  $\Lambda_{l,m}$ :

$$\Lambda_{l,m} = A''_{l,m} \tilde{c}_0(p, l, m) \quad (25)$$

with

$$A''_{l,m} = \frac{2^{2p(2m-1)+2} (2l+1)^p \Gamma(mp+1)^2}{\pi^{2p-1} \Gamma(2mp+2)} \left[ \frac{\Gamma(m + \frac{1}{2})^2 \Gamma(m+1)^2 \Gamma(l-m+1) \Gamma(l+m+1)}{\Gamma(2m+1)^2 \Gamma(l+1)^2} \right]^p, \quad (26)$$



and

$$\begin{aligned} \tilde{c}_0(p, l, m) &= \binom{l}{l-m}^{2p} \sum_{j_1, \dots, j_{2p}=0}^{l-m} \frac{(mp+1)_{j_1+\dots+j_{2p}}}{(2mp+2)_{j_1+\dots+j_{2p}}} \\ &\times \frac{(m-l)_{j_1} (l+m+1)_{j_1} \cdots (m-l)_{j_{2p}} (l+m+1)_{j_{2p}}}{(m+1)_{j_1} \cdots (m+1)_{j_{2p}} j_1! \cdots j_{2p}!}. \end{aligned} \quad (27)$$

Then, taking (25) into (8) one finally obtains the value

$$R_p[Y_{l,m}] = \frac{1}{1-p} \ln [A''_{l,m} \tilde{c}_0(p, l, m)]. \quad (28)$$

for the angular part for the Rényi entropy of any quantum state of an arbitrary central potential, which again hold for positive integer and half-integer values of the parameter  $p$ . Note that Eqs. (26) - (28) allow us to analytically compute this entropic quantity in a straightforward and algorithmic way.

### B. Bell-polynomials-based method

Let us now give an alternative, qualitatively different method to compute the angular Rényi functional  $\Lambda_{l,m}$  given by (18) or, equivalently, (20). In this method we calculate the Gegenbauer-polynomial integral involved in (18), or better the Jacobi-polynomial integral of (20), by means of the power expansion of its respective kernel. The latter is done by use of the following general result [44]: The  $p$ -th power of an arbitrary polynomial  $y_n(x)$  given by

$$y_n(x) = \sum_{k=0}^n c_k x^k \quad (29)$$

can be expressed as

$$\begin{aligned} [y_n(x)]^p &= \left( \sum_{k=0}^n c_k x^k \right)^p \\ &= \sum_{k=0}^{np} A_{k,p}(c_0, \dots, c_n) x^k, \end{aligned} \quad (30)$$

where

$$A_{k,p}(c_0, \dots, c_n) = \frac{p!}{(k+p)!} B_{k+p,p}(c_0, 2!c_1, \dots, (k+1)!c_k),$$

with  $c_i = 0$  if  $i > n$  and  $B_{n,k}(x_1, x_2, \dots)$  are the multivariate Bell polynomials of the second kind [46]

$$B_{n,k}(x_1, x_2, \dots) = \sum_{\substack{j_1+j_2+\dots+j_k=k \\ j_1+2j_2+\dots=n}} \frac{n!}{j_1!j_2!\cdots} \left(\frac{x_1}{1!}\right)^{j_1} \left(\frac{x_2}{2!}\right)^{j_2} \cdots$$

From the known explicit expression of the Jacobi polynomials [67] we can write

$$\tilde{P}_n^{(\alpha,\beta)}(x) = \sum_{k=0}^n c_k x^k \quad (31)$$

with the expansion coefficients

$$c_k = \sqrt{\frac{\Gamma(n+\alpha+1)(2n+\alpha+\beta+1)}{n!2^{\alpha+\beta+1}\Gamma(\alpha+\beta+n+1)\Gamma(n+\beta+1)}} \sum_{i=k}^n (-1)^{i-k} \binom{n}{i} \binom{i}{k} \frac{\Gamma(\alpha+\beta+n+i+1)}{2^i \Gamma(\alpha+i+1)}$$

Then, according to (30) et sequel one obtains the following expression for the  $p$ -th power of the orthonormal Jacobi polynomials

$$[\tilde{P}_n^{(\alpha,\beta)}(x)]^{2p} = \sum_{k=0}^{2np} B_{k+2p,2p}(c_0, 2!c_1, \dots, (k+1)!c_k)x^k. \quad (32)$$

Now, using this expression with  $\alpha = \beta = m$  and  $n = l - m$ , and taking the resulting expression into the angular functional  $\Lambda_{l,m}$  given by (20) one has

$$\begin{aligned} \Lambda_{l,m} &= \frac{\Gamma(mp+1)}{2^p \pi^{p-1}} \sum_{k=0}^{2(l-m)p} \frac{(2p)!}{(k+p)!} B_{k+2p,2p}(c_0, 2!c_1, \dots, (k+1)!c_k) \frac{[1 + (-1)^k] \Gamma(\frac{k+1}{2})}{\Gamma(\frac{1}{2}(3+k+2mp))} \\ &\equiv \frac{\Gamma(mp+1)}{2^p \pi^{p-1}} \Sigma(l, m, p). \end{aligned} \quad (33)$$

Thus, from (8) one finds the following value

$$R_p[Y_{l,m}] = \frac{1}{1-p} \ln \Lambda_{l,m} \frac{1}{1-p} \ln \left[ \frac{\Gamma(mp+1)}{2^p \pi^{p-1}} \Sigma(l, m, p) \right]. \quad (34)$$

for the angular Rényi entropy of an arbitrary state  $(l, m)$  of any central potential  $V(r)$ , which holds for positive integer and half-integer values of the parameter  $p$ .

Let us finally calculate, for illustration, both the angular Rényi and Shannon entropies for some specific states by means of Eqs. (34) and (12).

1. **States**  $(l, l)$ . From its own definition (18) one finds the angular functional

$$\begin{aligned} \Lambda_{l,l} &= 2\pi (A_{l,l})^{2p} \int_0^\pi (\sin \theta)^{2l+1} d\theta \\ &= \frac{2^{(2l-1)p+1} (l + \frac{1}{2})^p \Gamma(l + \frac{1}{2})^{2p} \Gamma(lp+1)}{\pi^{2p-\frac{3}{2}} \Gamma(2l+1)^p \Gamma(lp + \frac{3}{2})}, \end{aligned} \quad (35)$$

which holds for all real values of  $p$ . Then, from (8) one finds that the angular Rényi entropy of the state  $(l, l)$  is given by

$$R_p[Y_{l,l}] = \frac{1}{1-p} \times \ln \left[ \frac{2^{(2l-1)p+1} (l + \frac{1}{2})^p \Gamma(l + \frac{1}{2})^{2p} \Gamma(lp+1)}{\pi^{2p-\frac{3}{2}} \Gamma(2l+1)^p \Gamma(lp + \frac{3}{2})} \right], \quad (36)$$

Then, from this expression and (11) one has the following value

$$S[Y_{l,l}] = -l \left[ \psi(l+1) - \psi\left(l + \frac{3}{2}\right) + \ln 4 \right] + \ln \frac{4\pi^2}{2l+1} + \ln \frac{\Gamma(2l+1)}{\Gamma(l + \frac{1}{2})^2}, \quad (37)$$

for the angular Shannon entropy of the state  $(l, l)$ .

In particular, for the states  $(0, 0)$  and  $(1, 1)$  we have that

$$\Lambda_{0,0} = (4\pi)^{1-p}$$

and

$$\Lambda_{1,1} = \frac{2^{1-3p} 3^p \pi^{\frac{3}{2}-p} \Gamma(p+1)}{\Gamma(p + \frac{3}{2})},$$

so that the corresponding angular Rényi entropies are given by

$$R_p[Y_{0,0}] = \ln(4\pi)$$

and

$$R_p[Y_{1,1}] = \frac{1}{1-p} \ln \left[ \frac{2^{1-3p} 3^p \pi^{\frac{3}{2}-p} \Gamma(p+1)}{\Gamma(p+\frac{3}{2})} \right],$$

respectively, which both hold for all real values of  $p$ . Then, taking the limit  $p \rightarrow 1$  in the two previous expressions leads us to the following values

$$\begin{aligned} S[Y_{0,0}] &= \ln(4\pi) \\ S[Y_{1,1}] &= \ln\left(\frac{2\pi}{3}\right) + \frac{5}{3}, \end{aligned}$$

for the angular Shannon entropies of the states  $(0,0)$  and  $(1,1)$ , respectively.

2. **States**  $(l, l-1)$ . Operating similarly as in the previous case, one has the angular functional

$$A_{l,l-1} = 2\pi \left( \frac{(l+\frac{1}{2})(2l-1)^2 \Gamma(l-\frac{1}{2})^2}{2^{3-2l}(2l-1)! \pi^2} \right)^p \frac{\Gamma(p+\frac{1}{2}) \Gamma(pl-p+1)}{\Gamma(pl+\frac{3}{2})}$$

(which holds for all real values of  $p$ ) so that the angular Rényi entropy is given by

$$R_p(Y_{l,l-1}) = \frac{1}{1-p} \ln A_{l,l-1}$$

and the limit  $p \rightarrow 1$  gives rise to the value

$$S(Y_{l,l-1}) = -\ln \left( \frac{(l+\frac{1}{2})(2l-1)^2 \Gamma(l-\frac{1}{2})^2}{2^{3-2l}(2l-1)! \pi^2} \right) - \psi\left(\frac{3}{2}\right) - (l-1)\psi(l) + l\psi\left(l+\frac{3}{2}\right) \quad (38)$$

for the angular Shannon entropy. For the particular case  $(1,0)$ , one has the angular functional

$$\begin{aligned} \Lambda_{1,0} &= 2\pi \left(\frac{3}{4\pi}\right)^p \int_0^\pi |\cos\theta|^{2p} \sin\theta \, d\theta \\ &= \frac{3^p (4\pi)^{1-p}}{2p+1} \end{aligned}$$

and the following values

$$\begin{aligned} R_p[Y_{1,0}] &= \frac{1}{1-p} \ln \left[ \frac{3^p (4\pi)^{1-p}}{2p+1} \right], \\ S[Y_{1,0}] &= \frac{2}{3} + \ln\left(\frac{4\pi}{3}\right). \end{aligned}$$

for the angular Rényi and Shannon entropies.

#### IV. RÉNYI AND SHANNON ENTROPIES OF RYDBERG-LIKE HARMONIC STATES

In this section, we first determine the radial part of the position Rényi and Shannon entropies for the highly-energetic (Rydberg) states of the (three-dimensional) isotropic harmonic oscillator from their corresponding definitions (7) and (11). Then the resulting radial values together with the angular values derived in the previous section allows us to calculate the total Rényi and Shannon entropies (as well as the Tsallis ones, because of Eq. (2)) of the Rydberg harmonic states, what is illustrated for some specific oscillator-like states.

##### A. Radial Rényi entropies

Taking into account (7) and (15), the radial Rényi entropy of a general oscillator-like state can be expressed as

$$R_p[\rho_{n,l}] = \frac{1}{1-p} \ln \left[ (2\lambda^{3/2})^{p-1} N_{n,l}(p) \right], \quad (39)$$

where  $N_{n,l}(p)$  denotes the  $\mathfrak{L}_p$ -norm of the Laguerre polynomials given by

$$N_{n,l}(p) = \int_0^\infty \left( \left[ \widehat{L}_n^{(\alpha)}(x) \right]^2 w_\alpha(x) \right)^p x^\beta dx, \quad p > 0, \quad (40)$$

where  $\alpha = l + \frac{1}{2}$ ,  $l = 0, 1, 2, \dots$  and  $\beta = \frac{1}{2}(1 - p)$ . We note that the condition

$$\beta + p\alpha = pl + \frac{1}{2} > -1, \quad (41)$$

guarantees the convergence of the integral (40) at zero, i.e., is always satisfied for physically meaningful values of the parameters  $\alpha$ ,  $\beta$  and  $p$ .

Then, the problem of determination of the radial Rényi entropy of a general oscillator-like state boils down to the study of the asymptotics ( $n \rightarrow \infty$ ) of the Laguerre norm  $N_{n,l}(p)$ . The latter problem can be solved by means of the recent methodology of Aptekarev et al [4], which takes explicitly into account the different asymptotical representations for the Laguerre polynomials at different regions of the real half-line.

Moreover, this technique shows that the dominant contribution in the magnitude of the integral comes from various regions of integration in (40), which depend on the different values of the involved parameters ( $\alpha, p, \beta$ ). In fact, there are five asymptotical regimes which can give (depending on  $\alpha, \beta$  and  $p$ ) the dominant contribution in the asymptotics of  $N_n(\alpha, p, \beta)$ . First, at the neighborhood of zero (Bessel regime) the Laguerre polynomials can be asymptotically described by means of Bessel functions. Then, to the right of zero (in the bulk region of zeros location) the oscillatory behavior of the polynomials is asymptotically modelled via trigonometric functions (cosine regime). And at the neighborhood of the extreme right (Airy regime), the zeros asymptotics is given by Airy functions. Finally, at the extreme right of the orthogonality interval (i.e., near infinity) the polynomials have growing asymptotics. Moreover, there are two transition regions (to be called by cosine-Bessel and cosine-Airy) where these asymptotics match each other; i.e., asymptotics of the Bessel functions for big arguments match the trigonometric function, as well as the asymptotics of the Airy functions do the same.

The application of Aptekarev et al' technique to the Laguerre norm (40) in our three-dimensional case, together with Eq. (39), gives rise to the following value for the radial Rényi entropy of the Rydberg harmonic states:

$$R_p[\rho_{n,l}] = \begin{cases} \frac{1}{1-p} \ln \left[ \lambda^{\frac{3}{2}(p-1)} C(\beta, p) (2n^3)^{\frac{1-p}{2}} (1 + \bar{o}(1)) \right], & p \in (0, p^*) \\ -2 \ln \left[ \lambda^{3/4} \frac{8\sqrt{2}}{3\pi^{5/2}} n^{-3/4} (\ln n + \underline{O}(1)) \right], & p = p^* \\ \frac{1}{1-p} \ln \left[ (2\lambda^{\frac{3}{2}})^{p-1} C_B(\alpha, \beta, p) n^{(p-3)/2} (1 + \bar{o}(1)) \right], & p > p^* \end{cases}, \quad (42)$$

with  $p^* = \frac{3}{2}$  and the constants  $C$  and  $C_B$  are defined as

$$C_B(\alpha, \beta, p) := 2 \int_0^\infty t^{2\beta+1} |J_\alpha(2t)|^{2p} dt. \quad (43)$$

for the Bessel regime,

$$C(\beta, p) := \frac{2^{\beta+1}}{\pi^{p+1/2}} \frac{\Gamma(\beta + 1 - p/2) \Gamma(1 - p/2) \Gamma(p + 1/2)}{\Gamma(\beta + 2 - p) \Gamma(1 + p)}. \quad (44)$$

for the cosine regime, respectively (the symbol  $J_\alpha(z)$  denotes the Bessel function, see e.g. [67]), and the parameters  $\alpha \equiv \alpha(l)$  and  $\beta \equiv \beta(p)$  are given by (41).

*Hints:* To better understand the application of the previous technique to our case, let us note:

- that  $\beta(p^*) - \frac{p^*}{2} = \frac{1}{2} - p^* = -1$ , so that from (44) we have  $C(\beta, p) = \infty$ . Thus, for  $p \in (0, p^*)$  the region of  $\mathbb{R}_+$  where the Laguerre polynomials exhibit the cosine asymptotics contributes with the dominant part in the integral (40). For  $p = p^*$  the transition cosine-Bessel regime determines the asymptotics of  $N_{n,l}(p^*)$ , and for  $p > p^*$  the Bessel regime plays the main role.

- the  $\mathfrak{L}_p$ -norm is constant (i.e., independent of  $n$ ) and equal to  $C_B(\alpha, \beta, p)$ , only when  $(p-1)3/2 - p = 0$ . This means that the constancy occurs when  $p = 3$ .

A careful analysis of (42) shows that:

- for fixed  $n$  the radial entropy depends on the oscillator strength  $\lambda$  in the form  $-3/2 \ln \lambda$ ,
- for fixed  $\lambda$  the radial entropy depends on the principal quantum number  $n$  in the forms:  $3/2 \ln n$  (as  $p \in ]0, 3/2[$ ,  $+3/2 \ln n - 2 \ln \ln n$  (as  $p = 3/2$ ), constant (as  $p = 3$ ), and  $\frac{p-3}{2(1-p)} \ln n$  (as  $p > 3$ ).

Since the Rényi and Tsallis entropies are related by (2), the radial Tsallis entropy,  $T_p[\rho_{n,l}]$ , for the Rydberg oscillator-like states follows from (42) in a straightforward manner.

### B. Radial Shannon entropy

To determine the radial part of the Shannon entropy  $S[\rho_{n,l}]$  we need, according to (11), to compute the limit  $p \rightarrow 1$  of the radial Rényi entropy  $R_p[\rho_{n,l}]$  given by (42). We obtain that

$$\begin{aligned} S[\rho_{n,l}] &\equiv \lim_{p \rightarrow 1} R_p[\rho_{n,l}] \\ &= \lim_{p \rightarrow 1} \frac{1}{1-p} \ln \left[ \lambda^{\frac{3}{2}(p-1)} C(\beta, p) (2n^3)^{\frac{1-p}{2}} (1 + \bar{o}(1)) \right] \\ &= \left( \frac{3}{2} \ln n - \frac{3}{2} \ln \lambda + \ln \pi - 1 \right) (1 + \bar{o}(1)), \end{aligned} \quad (45)$$

where it can be seen that the leading term of the asymptotic expression is proportional to  $\ln n$ , as expected.

### C. Total position Rényi and Shannon entropies

The total Rényi and Shannon entropies of the Rydberg harmonic states  $\{n \rightarrow \infty, l, m\}$ , given by Eqs. (6) and (10) respectively, can now be determined from the results obtained in the two previous sections in a direct, analytical and straightforward manner. Indeed they are given by the sum of the angular part (which does not depend on  $n$ ) obtained in section III in two different ways and the radial part which is given by Eqs. (42) and (45) for the Rényi and Shannon entropies, respectively. When  $n$  is sufficiently large, we observe that :

1. If  $p \neq 3$ , then  $|R_p[\rho_{n,l}]| \gg |R_p[Y_{l,m}]|$ , and so  $R_p[\rho_{n,l,m}] \simeq R_p[\rho_{n,l}] \rightarrow \pm\infty$  with the same sign that  $3-p$ . This  $n$ th-asymptotical growth of the absolute value of the radial part is very very slow; the closer  $p$  to 3, the slower is this growth.
2. If  $p = 3$ , then  $R_p[\rho_{n,l}]$  does not depend on  $n$  and so  $R_p[\rho_{n,l,m}] = R_p[\rho_{n,l}] + R_p[Y_{l,m}]$ , where the two summands are given by Eqs. (42) and (28) or (34), respectively.

In particular, we have obtained the values

$$R_p[\rho_{n,0,0}] = R_p[\rho_{n,0}] + R_p[Y_{0,0}] \begin{cases} \simeq R_p[\rho_{n,0}] \rightarrow +\infty, & p \in ]0, 3[ \\ = \ln(4\pi) - \frac{1}{2} \ln[4\lambda^3 C_B(\alpha, -1, 3)], & p = 3 \\ \simeq R_p[\rho_{n,0}] \rightarrow -\infty, & p > 3 \end{cases}, \quad (46)$$

for the total Rényi entropy of the state  $(n \rightarrow \infty, 0, 0)$ , and the values

$$R_p[\rho_{n,1,0}] = R_p[\rho_{n,1}] + R_p[Y_{1,0}] \begin{cases} \simeq R_p[\rho_{n,1}] \rightarrow +\infty, & p \in ]0, 3[ \\ = \frac{1}{1-p} \ln \left[ \frac{3^p (4\pi)^{1-p}}{2^{p+1}} \right] - \frac{1}{2} \ln[4\lambda^3 C_B(\alpha, -1, 3)], & p = 3 \\ \simeq R_p[\rho_{n,1}] \rightarrow -\infty, & p > 3 \end{cases}, \quad (47)$$

for the total Rényi entropy of the state ( $n \rightarrow \infty, 1, 0$ ). Note that the radial entropies  $R_p[\rho_{n,0}]$  and  $R_p[\rho_{n,1}]$  in Eqs. (46) and (47), respectively, can be easily derived from (42) with  $\beta = 1/2(1-p)$  and  $\alpha = 1/2, 3/2$ , respectively. From these results (46) and (47) it can be easily shown that the Shannon entropy and the disequilibrium grow as  $3/2 \ln n$  and  $1/2 \ln n$ , respectively.

## V. POSITION-MOMENTUM RÉNYI AND SHANNON UNCERTAINTY SUMS

In this section we illustrate that our entropy results for the states at both extreme regions of the oscillator's energetic spectrum satisfy the known entropic uncertainty relations based on the Shannon entropy [11, 12] and the Rényi entropy [13, 14]. We begin by taking into account that, as already pointed out at the end of Section II, the quantum probability densities in the position and momentum spaces of our system are related through

$$\gamma_{n,l,m}(\vec{p}) = \frac{1}{\lambda^3} \rho_{n,l,m} \left( \frac{\vec{p}}{\lambda} \right), \quad (48)$$

so that the Rényi entropy in momentum space can be obtained from the position entropy as

$$R_p[\gamma_{n,l,m}] = R_p[\rho_{n,l,m}] + 3 \ln \lambda, \quad p \neq 1. \quad (49)$$

Then, for the  $ns$ -states (i.e., states with  $l = m = 0$ ) we have that the joint position-momentum Rényi-entropy-based uncertainty sum has the value

$$R_p[\rho_{n,0,0}] + R_q[\gamma_{n,0,0}] = \ln \left\{ [N_{n,0}(q)]^{\frac{1}{1-q}} [N_{n,0}(p)]^{\frac{1}{1-p}} \right\} + 2 \ln(2\pi), \quad \frac{1}{p} + \frac{1}{q} = 2, \quad \forall (n, 0, 0). \quad (50)$$

(where we have taken into account Eqs. (39) and (49)). In particular, this expression gives the value

$$R_p[\rho_{0,0,0}] + R_q[\gamma_{0,0,0}] = \ln \left[ \left( \frac{\pi^{\frac{1-p}{2}}}{p^{3/2}} \right)^{\frac{1}{1-p}} \left( \frac{\pi^{\frac{1-q}{2}}}{q^{3/2}} \right)^{\frac{1}{1-q}} \right] + 2 \ln \pi, \quad (51)$$

for the ground state  $(n, l, m) = (0, 0, 0)$  of the harmonic oscillator, which saturates the Bialynicki-Birula-Zozor-Vignat Rényi-entropy-based uncertainty relation [13, 14]. Moreover, for  $p \rightarrow 1$  and  $q \rightarrow 1$ , this expression gives the value

$$S[\rho_{0,0,0}] + S[\gamma_{0,0,0}] = 3(1 + \ln \pi), \quad (52)$$

for the joint Shannon uncertainty sum of the oscillator ground-state, which saturates the celebrated Shannon-entropy uncertainty relation of Bialynicki-Birula and Mycielski [11]. Starting with Eqs. (46) and operating in a similar way we can obtain the corresponding expressions for the position and momentum Rényi and Shannon entropies of the Rydberg oscillator-like states ( $n \rightarrow \infty, 0, 0$ ), which again verify the Rényi-entropy-based and Shannon-entropy-based uncertainty relations.

Moreover, let us now consider the oscillator states  $(n, l, m) = (1, l, 0)$ . Then, one has that the joint Rényi-entropy-based uncertainty sum is

$$R_p[\rho_{1,l,0}] + R_q[\gamma_{1,l,0}] = R_p[\rho_{1,l}] + R_q[\gamma_{1,l}] + R_p[Y_{l,0}] + R_q[Y_{l,0}] \quad (53)$$

which, taking into account Eq. (39), transforms into

$$R_p[\rho_{1,l,0}] + R_q[\gamma_{1,l,0}] = \ln \left\{ [N_{1,l}(p)]^{\frac{1}{1-p}} [N_{1,l}(q)]^{\frac{1}{1-q}} \right\} + R_p[Y_{l,0}] + R_q[Y_{l,0}] - 2 \ln 2, \quad (54)$$

where the radial integral can be shown (see the Appendix A) to have the value

$$N_{1,l}(p) = \frac{\Gamma(lp + \frac{3}{2})}{\Gamma(l + \frac{5}{2})^p} \frac{(2p)!}{p^{(l+2)p + \frac{3}{2}}} L_{2p}^{(-(l+2)p - \frac{3}{2})} \left( - \left( l + \frac{3}{2} \right) p \right), \quad (55)$$

In particular for states with  $l = 0$ , since  $R_p[Y_{0,0}] = \ln(4\pi)$ , one has from Eq. (54) that

$$R_p[\rho_{1,0,0}] + R_q[\gamma_{1,0,0}] = \ln \left\{ [N_{1,0}(p)]^{\frac{1}{1-p}} [N_{1,0}(q)]^{\frac{1}{1-q}} \right\} + 2 \ln(2\pi), \quad (56)$$

where the integral  $N_{1,0}(p)$  can be easily obtained from Eq. (56). Now, it is straightforward to check that this value verifies the Rényi-entropy-based uncertainty relation. Finally, let us point out that starting with Eqs. (42), (49) and (50) and operating similarly we can readily see that the joint Rényi uncertainty sum of the Rydberg states ( $n \rightarrow \infty, 1, 0$ ) satisfy this entropic uncertainty relation as well.

## VI. CONCLUSIONS

The harmonic systems are possibly the best studied finite systems in quantum physics since their wave equation can be exactly solved and because of their so many useful applications in science and technology. However, the knowledge of their information-theoretic measures is scarce and little known. Indeed, the spreading or spatial extension of the quantum-mechanical density of the isotropic harmonic oscillator has been examined by means of their central moments, particularly the second one (i.e., the variance) [10], almost up until now. However, their entropic measures (which are much more adequate to quantify the density of the oscillator-like states because they do not depend on any specific point of the system's region, contrary to what happens with the moments about the origin and the central moments) have been scarcely studied [3, 37, 39, 70–72] and their determination is yet incomplete. This work has partially filled up this lack in the two following analytical ways.

We have determined the angular part of the basic entropic measures (Rényi, Tsallis, Shannon, disequilibrium) of the single-particle probability density which characterize the quantum states of ANY central potential. Then, we have computed the values of the total (i.e., angular+radial parts) values of these entropies for the highly-energetic oscillator-like states whose utility and multidirectional relevance is well-known. Finally we have performed the analytical calculation of the dominant term of the radial part in the Rydberg case, what is specially remarkable because it is a serious problem even numerically. Indeed, a naive use of quadratures for the numerical evaluation of the involved entropic functionals of the Laguerre polynomials which control the harmonic states is not convenient because the increasing number of integrable singularities spoil any attempt to achieve reasonable accuracy even for rather small values of  $n$ , since all the zeros of  $L_n(x)$  belong to the interval of orthogonality. Moreover, we have illustrated that the analytic determination of the information entropies of the low energy oscillator-like states is much simpler. Finally, we have shown that the entropy results obtained for the joint position-momentum uncertainty sum at both extreme regions of the harmonic energetic spectrum satisfy the known Shannon-entropy-based and Rényi-entropy-based uncertainty relations.

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### Appendix A: Derivation of Equation (55)

To obtain Eq.(55) we start with the well-known [67] Euler's integral of the second kind  $\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt$ ,  $\text{Re}(z) > 0$ , which can be easily extended as

$$\int_0^\infty x^{\nu-1} e^{-\mu(x+a)} dx = \Gamma(\nu) \frac{e^{-\mu a}}{\mu^\nu}, \quad \mu > 0, \nu > 0, a \in \mathbb{R}.$$

Now, the  $n$ th-derivative with respect to  $\mu$  in this expression and taking into account the Rodrigues' formula of the Laguerre polynomials allow us to have that

$$\int_0^\infty (a+x)^n x^{\nu-1} e^{-\mu x} dx = (-1)^n \Gamma(\nu) \cdot e^{\mu a} \frac{d^n}{d\mu^n} (e^{-\mu a} \mu^{-\nu}) = (-1)^n \frac{\Gamma(\nu)n!}{\mu^{n+\nu}} L_n^{(-n-\nu)}(a\mu), \quad (\text{A1})$$

which can be rewritten as

$$L_n^{(-n-\nu)}(x) = \frac{(-1)^n}{n! \Gamma(\nu)} \int_0^\infty (x+y)^n y^{\nu-1} e^{-y} dy, \quad (\text{A2})$$

which gives an integral representation for the varying Laguerre polynomials with a negative parameter, what is interesting *per se* in the field of orthogonal polynomials. Finally, for the particular case  $2p \in \mathbb{N}$ , we can insert (A1) into (40) to obtain the wanted expression

$$N_{1,l}(p) = \frac{\Gamma(lp + \frac{3}{2})}{\Gamma(l + \frac{5}{2})^p} \frac{(2p)!}{p^{(l+2)p + \frac{3}{2}}} L_{2p}^{(-(l+2)p - \frac{3}{2})} \left( - \left( l + \frac{3}{2} \right) p \right), \quad (\text{A3})$$

which holds for the states with  $(n = 1, l = 0)$  and  $(n = 1, l = 1)$ .

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## 3.2 High-dimensional states

There has been a permanent interest for multidimensional harmonic systems since the very early times of quantum physics, as can be seen e.g. in general quantum mechanics [11, 170, 183–193], quantum chromodynamics and elementary particle physics [147, 194], atomic and molecular physics [195, 196], heat transport [197–199], information theory [37, 122, 174, 178, 200], fractality [200] and entanglement [201, 202]. This system is closely related to completely classical periodic systems in Nature. In elementary particle physics, we encounter many oscillating modes whose energy packets are the fundamental particles which may be linked to periodic structures in a classical underlying theory [194]. Moreover, a rather comprehensive analysis of thermodynamic properties of the multidimensional harmonic system obeying the Polychronakos fractional statistics with a complex parameter has been recently given [200].

Then, it is amazing that the information-theoretic properties of multidimensional harmonic systems is very poorly known in spite of a few efforts [37, 122, 122, 173, 174, 177]. In this section we fill up this information lack by determining in an analytical way the Rényi entropies with a natural parameter for the high-dimensional (pseudo-classical) states of the  $D$ -dimensional harmonic system in position and momentum spaces and their associated uncertainty relations in terms of the basic parameters which characterize the system. This goal has been achieved by use of modern asymptotical methods of the hypergeometric orthogonal polynomials described in Section 1.2, which control the harmonic stationary states of our system, and other special functions of Applied Mathematics and Mathematical Physics.

The following specific tasks for the high-dimensional (pseudo-classical) states of the  $D$ -dimensional harmonic system have been carried out:

- Determination of the Heisenberg-like uncertainty measures as given by the position and momentum radial expectation values at the high  $D$  limit.
- Calculation of the Rényi entropies with natural parameter at the high  $D$  limit in the two conjugated position and momentum spaces.
- Determination of the associated Heisenberg-like uncertainty products and Rényi-like uncertainty sums, showing that they not only fulfill the general Heisenberg-like and entropic uncertainty relations but also they exhaust them.
- We conjecture the leading term of the Shannon entropy at the high  $D$  limit.

These results have been published in the article [65] with coordinates: **Puertas-Centeno D.**, Toranzo I. V. and Dehesa, J. S. *Heisenberg and entropic uncertainty measures for large-dimensional harmonic systems*. Entropy, 19:164, 2017, which is attached below.

# Heisenberg and entropic uncertainty measures for large-dimensional harmonic systems

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The  $D$ -dimensional harmonic system (i.e., a particle moving under the action of a quadratic potential) is, together with the hydrogenic system, the main prototype of the physics of multidimensional quantum systems. In this work we rigorously determine the leading term of the Heisenberg-like and entropy-like uncertainty measures of this system as given by the radial expectation values and the Rényi entropies, respectively, at the limit of large  $D$ . The associated multidimensional position-momentum uncertainty relations are discussed, showing that they saturate the corresponding general ones. A conjecture about the Shannon-like uncertainty relation is given and an interesting phenomenon is observed: the Heisenberg-like and Rényi-entropy-based equality-type uncertainty relations for all the  $D$ -dimensional harmonic oscillator states in the pseudoclassical ( $D \rightarrow \infty$ ) limit are the same as the corresponding ones for the hydrogenic systems, despite the so different character of the oscillator and Coulomb potentials.

Keywords: Entropic uncertainty measures;  $D$ -dimensional harmonic oscillator;  $D$ -dimensional quantum physics; radial and momentum expectation values; harmonic states at large dimensions

## I. INTRODUCTION

Various analytically solvable continuous models with standard and non-standard dimensionalities have been shown to be very effective in the description of quantum dots, ultracold gases in harmonic traps, fractional quantum Hall effect and quark confinement. This is the case of the N-Harmonium (N harmonically interacting fermions in a harmonic trap) [1, 2], the Spherium (two electrons trapped on the surface of a sphere) [3–5], the Hooke atom (a pair of electrons repelling Coulombically and confined by a harmonic external potential) [6, 7], the Crandall-Whitney-Bettega system (a two-electron atom with harmonic confinement plus inverse square law interparticle repulsion) [8] and the celebrated Moshinsky [9, 10] and Calogero-Moser-Sutherland models [12]. These models have long been regarded as an important laboratory toolbox in numerous scientific fields from quantum chemistry to quantum information, mainly because they are completely integrable analogues of many body systems due to their remarkable analytic properties.

Moreover, Herschbach et al [13, 14] and other authors (see the review [15]) have designed a very useful strategy, the dimensional scaling method, to solve the atomic and molecular systems not in the standard three-dimensional framework (where they possess an  $O(3)$  rotation symmetry) but in a  $D$ -dimensional theory, so that the symmetry is  $O(D)$ . This method allows to solve a finite many-body problem in the ( $D \rightarrow \infty$ )-limit and then perturbation theory in  $1/D$  is used to have an approximate result for the standard dimension ( $D = 3$ ), obtaining at times a quantitative accuracy comparable to or better than single-zeta Hartree-Fock calculations [13, 14, 16].

The main point here is that for electronic structure the ( $D \rightarrow \infty$ )-limit is beguilingly simple and exactly computable for any atom and molecule. For  $D$  finite but very large, the electrons are confined to harmonic oscillations about the fixed positions attained in the ( $D \rightarrow \infty$ )-limit. Indeed, in this limit the electrons of a many-electron system assume fixed positions relative to the nuclei and each other, in the  $D$ -scaled space. Moreover, the large- $D$  electronic geometry and energy correspond to the minimum of an exactly known effective potential and can be determined from classical electrostatics for any atom or molecule. The ( $D \rightarrow \infty$ )-limit is called *pseudoclassical*, tantamount to  $\hbar \rightarrow 0$  and/or  $m_e \rightarrow \infty$  in the kinetic energy, being  $\hbar$  and  $m_e$  the Planck constant and the electron mass, respectively. This limit is not the same as the conventional classical limit obtained by  $\hbar \rightarrow 0$  for a fixed dimension [17, 18]. Although at first sight the electrons at rest in fixed locations might seem violate the uncertainty principle, this is not true because that occurs only in the  $D$ -scaled space (see e.g., [19]).

The dimensional scaling method has been mainly applied to Coulomb systems but not yet to harmonic systems to the best of our knowledge. This is highly surprising because of the huge interest for  $D$ -dimensional harmonic oscillators in general quantum mechanics [20–32], quantum chromodynamics and elementary particle physics [33, 34], atomic and molecular physics [35, 36], heat transport [37–39], information theory [40–44], fractality [43] and entanglement [45, 46]. Moreover, the  $D$ -dimensional quantum harmonic oscillator is closely related to completely classical periodic systems in Nature. In elementary particle physics, we encounter many oscillating modes whose energy packets are the fundamental particles which may be linked to periodic structures in a classical underlying

theory [33]. In addition, a recent effort [43] has given a rather comprehensive analysis of thermodynamic properties of a  $D$ -dimensional harmonic oscillator system obeying the Polychronakos fractional statistics with a complex parameter.

Despite this increasing interest from both theoretical and applied standpoints, there does not exist a deep knowledge about the Heisenberg and entropy-like uncertainty measures of the  $D$ -dimensional harmonic oscillator (i.e., a particle moving under the action of a quadratic potential) in the quantum-pseudoclassical border although a few works have been carried out [21, 40, 47–58]. These measures, which quantify the spreading properties of the harmonic probability density, are respectively characterized by the radial expectation values and the Rényi and Shannon entropies of the corresponding quantum probability density of the system in position and momentum spaces. Lately, two efforts have been able in the last few months to determine these uncertainty measures of the main prototype of the  $D$ -dimensional Coulomb systems (namely, the  $D$ -dimensional hydrogenic atom [59]) at the pseudoclassical limit in an analytically compact way [60, 61]. A similar work for the  $D$ -dimensional harmonic system is the goal of the present paper.

The radial expectation values of the  $D$ -dimensional harmonic system in both position and momentum spaces have been formally found [55] in terms of  $D$ , the hyperquantum numbers of the harmonic states and the oscillator strength  $\lambda$  through a generalized hypergeometric function evaluated at unity  ${}_3F_2(1)$ , which cannot be easily calculated unless the hyperquantum numbers and/or the dimension  $D$  are sufficiently small; nevertheless the position and momentum expectation values of the lowest orders are explicitly known [48, 62].

The determination of the entropic measures of the  $D$ -dimensional harmonic oscillator, which describe most appropriately the electronic uncertainty of the system, is far more difficult except for the lowest-lying energy states despite some efforts [40, 41, 44, 47, 51–53, 63]. This is because these quantities are described by means of some power or logarithmic functionals of the electron density, which cannot be calculated in an analytical way nor numerically computed; the latter is basically because a naive numerical evaluation using quadratures is not convenient due to the increasing number of integrable singularities when the principal hyperquantum number  $n$  is increasing, which spoils any attempt to achieve reasonable accuracy even for rather small  $n$  [64]. Recently, the main entropic properties of the multi-dimensional highest-lying energy (i.e., Rydberg) harmonic states (namely, the Rényi, Shannon and Tsallis entropies) have been explicitly calculated in a compact form [44, 63] by use of modern techniques of approximation theory based on the strong asymptotics ( $n \rightarrow \infty$ ) of the Laguerre  $\mathcal{L}_n^{(\alpha)}(x)$  and Gegenbauer  $\mathcal{C}_n^{(\alpha)}(x)$  polynomials which control the state's wave functions in position and momentum spaces, respectively.

In this work we determine the position and momentum radial expectation values and the Rényi and Shannon entropies of the large-dimensional harmonic states in terms of the dimensionality  $D$ , the oscillator constant  $\lambda$  and the principal and orbital hyperquantum numbers of the states. The Rényi entropies  $R_q[\rho]$ ,  $q > 0$  are defined [65, 66] as

$$R_q[\rho] = \frac{1}{1-q} \log \int_{\mathbb{R}^3} [\rho(\vec{r})]^q d\vec{r}, \quad q \neq 1 \quad (1)$$

Note that the Shannon entropy  $S[\rho] = -\int \rho(\vec{r}) \log \rho(\vec{r}) d\vec{r} = \lim_{q \rightarrow 1} R_q[\rho]$ ; see e.g. [67, 68]. These quantities completely characterize the density  $\rho(\vec{r})$  [27, 69] under certain conditions. In fact, we can calculate from (1) other relevant entropic quantities such as e.g. the disequilibrium  $\langle \rho \rangle = \exp(R_2[\rho])$ , and the Tsallis [70] entropies  $T_q[\rho] = \frac{1}{q-1} (1 - \int_{\mathbb{R}^3} [\rho(\vec{r})]^q)$ , since  $T_q[\rho] = \frac{1}{1-q} [e^{(1-q)R_q[\rho]} - 1]$ . The properties of the Rényi entropies and their applications have been widely considered; see e.g. [66, 68, 71] and the reviews [72–74]. The use of Rényi and Shannon entropies as measures of uncertainty allow a wider quantitative range of applicability than the moments around the origin and the standard or root-square-mean deviation do. This permits, for example, a quantitative discussion of quantum uncertainty relations further beyond the conventional Heisenberg-like uncertainty relations [60, 73–75].

The structure of this work is the following. In section II the quantum-mechanical probability densities of the stationary states of the  $D$ -dimensional harmonic (oscillator-like) system are briefly described in both position and momentum spaces. In section III we determine the Heisenberg-like uncertainty measures of the large-dimensional harmonic system, as given by the radial expectation values of arbitrary order, in the two conjugated position and momentum spaces. They are calculated by use of some recent asymptotical results ( $\alpha \rightarrow \infty$ ) of the underlying Rényi-like integral functionals of the Laguerre polynomials  $\mathcal{L}_n^{(\alpha)}(x)$  and Gegenbauer polynomials  $\mathcal{C}_n^{(\alpha)}(x)$  which control the harmonic wavefunctions. The associated Heisenberg-like uncertainty products of the system are explicitly found and shown to satisfy the multidimensional Heisenberg uncertainty relationships for general quantum systems. In section IV we determine the Rényi entropies of the  $D$ -dimensional harmonic system at large  $D$  in both position and momentum spaces by means of the same asymptotical methodology. The dominant term of the associated position-momentum uncertainty sum for the general states of the large dimensional harmonic systems is also given and shown to fulfill the known position-momentum Rényi-entropy-based uncertainty relations [83–85]. Finally, some concluding remarks and open problems are given.

## II. THE $D$ -DIMENSIONAL HARMONIC PROBLEM: BASICS

In this section we briefly summarize the quantum-mechanical  $D$ -dimensional harmonic problem in both position and momentum spaces and we give the probability densities of the stationary quantum states of the system.

The time-independent Schrödinger equation of a  $D$ -dimensional ( $D \geq 1$ ) harmonic system (i.e., a particle moving under the action of the  $D$ -dimensional quadratic potential  $V(r) = \frac{1}{2}\lambda^2 r^2$ ) is given by

$$\left(-\frac{1}{2}\vec{\nabla}_D^2 + V(r)\right)\Psi(\vec{r}) = E\Psi(\vec{r}), \quad (2)$$

where  $\vec{\nabla}_D$  denotes the  $D$ -dimensional gradient operator,  $\lambda$  is the oscillator strength, and the position vector  $\vec{r} = (x_1, \dots, x_D)$  in hyperspherical units is given as  $(r, \theta_1, \theta_2, \dots, \theta_{D-1}) \equiv (r, \Omega_{D-1})$ ,  $\Omega_{D-1} \in S^{D-1}$ , where  $r \equiv |\vec{r}| = \sqrt{\sum_{i=1}^D x_i^2} \in [0, +\infty)$  and  $x_i = r \left(\prod_{k=1}^{i-1} \sin \theta_k\right) \cos \theta_i$  for  $1 \leq i \leq D$  and with  $\theta_i \in [0, \pi)$ ,  $i < D-1$ ,  $\theta_{D-1} \equiv \phi \in [0, 2\pi)$ . Atomic units (i.e.,  $\hbar = m_e = e = 1$ ) are used throughout the paper.

It is known (see e.g., [40, 76]) that the energies belonging to the discrete spectrum are given by

$$E = \lambda \left(2n + l + \frac{D}{2}\right) \quad (3)$$

(with  $n = 0, 1, 2, \dots$  and  $l = 0, 1, 2, \dots$ ) and the associated eigenfunction can be expressed as

$$\Psi_{n,l,\{\mu\}}(\vec{r}) = \mathcal{R}_{n,l}(r) \mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}), \quad (4)$$

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

$$\mathcal{R}_{n,l}(r) = \left(\frac{2n! \lambda^{l+\frac{D}{2}}}{\Gamma(n+l+\frac{D}{2})}\right)^{\frac{1}{2}} e^{-\frac{\lambda}{2}r^2} r^l \mathcal{L}_n^{(l+\frac{D}{2}-1)}(\lambda r^2). \quad (5)$$

The symbol  $\mathcal{L}_n^{(\alpha)}(x)$  denotes the orthogonal Laguerre polynomials [77] with respect to the weight  $\omega_\alpha(x) = x^\alpha e^{-x}$ ,  $\alpha = l + \frac{D}{2} - 1$ , on the interval  $[0, \infty)$ . The angular eigenfunctions are the hyperspherical harmonics,  $\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})$ , defined [40, 59, 78] as

$$\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) = \mathcal{N}_{l,\{\mu\}} e^{im\phi} \times \prod_{j=1}^{D-2} \mathcal{C}_{\mu_j - \mu_{j+1}}^{(\alpha_j + \mu_{j+1})}(\cos \theta_j) (\sin \theta_j)^{\mu_{j+1}} \quad (6)$$

with the normalization constant

$$\mathcal{N}_{l,\{\mu\}}^2 = \frac{1}{2\pi} \prod_{j=1}^{D-2} \frac{(\alpha_j + \mu_j)(\mu_j - \mu_{j+1})! [\Gamma(\alpha_j + \mu_{j+1})]^2}{\pi 2^{1-2\alpha_j-2\mu_{j+1}} \Gamma(2\alpha_j + \mu_j + \mu_{j+1})}, \quad (7)$$

with  $2\alpha_j = D - j - 1$  and where the symbol  $\mathcal{C}_m^{(\alpha)}(t)$  in Eq. (6) denotes the Gegenbauer polynomial [77] of degree  $m$  and parameter  $\alpha$ .

Note that the wavefunctions are duly normalized so that  $\int |\Psi_{n,l,\{\mu\}}(\vec{r})|^2 d\vec{r} = 1$ , where the  $D$ -dimensional volume element is  $d\vec{r} = r^{D-1} dr d\Omega_{D-1}$  where

$$d\Omega_{D-1} = \left(\prod_{j=1}^{D-2} (\sin \theta_j)^{2\alpha_j} d\theta_j\right) d\theta_{D-1},$$

and we have taken into account the normalization to unity of the hyperspherical harmonics given by  $\int |\mathcal{Y}_{l,\{\mu\}}(\Omega_D)|^2 d\Omega_D = 1$ . Then, the quantum probability density of a  $D$ -dimensional harmonic stationary state  $(n, l, \{\mu\})$  is given in position space by the squared modulus of the position eigenfunction given by (4) as

$$\rho_{n,l,\{\mu\}}(\vec{r}) = \rho_{n,l}(r) |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2, \quad (8)$$

where the radial part of the density is the univariate radial density function  $\rho_{n,l}(r) = [\mathcal{R}_{n,l}(r)]^2$ . On the other hand, the Fourier transform of the position eigenfunction  $\Psi_{n,l,\{\mu\}}(\vec{r})$  given by (4) provides the eigenfunction of the system in the conjugated momentum space,  $\tilde{\Psi}_{n,l,\{\mu\}}(\vec{p})$ . Then, we have the expression

$$\gamma_{n,l,\{\mu\}}(\vec{p}) = |\tilde{\Psi}_{n,l,\{\mu\}}(\vec{p})|^2 = \lambda^{-D} \rho_{n,l,\{\mu\}}\left(\frac{\vec{p}}{\lambda}\right). \quad (9)$$

for the momentum probability density of the  $D$ -dimensional harmonic stationary state with the hyperquantum numbers  $(n, l, \{\mu\})$ .

### III. RADIAL EXPECTATION VALUES OF LARGE-DIMENSIONAL HARMONIC STATES

In this section we obtain the radial expectation values of the  $D$ -dimensional harmonic state  $(n, l, \{\mu\})$  in the large- $D$  limit in both position and momentum spaces, denoted by  $\langle r^k \rangle$  and  $\langle p^t \rangle$ , respectively, with  $k$  and  $t = 0, 1, \dots$ . We start with the expressions (8) and (9) of the position and momentum probability densities of the system, respectively, obtaining the expressions

$$\begin{aligned} \langle r^k \rangle &= \int r^k \rho_{n,l,\{\mu\}}(\vec{r}) d\vec{r} = \int_0^\infty r^k \rho_{n,l}(x) r^{D-1} dr \int |\mathcal{Y}_{l,\{\mu\}}(\Omega_D)|^2 d\Omega_D \\ &= \int_0^\infty r^{k+D-1} \rho_{n,l}(x) dr \\ &= \frac{n! \lambda^{-k/2}}{\Gamma(n+l+D/2)} \int_0^\infty x^{\alpha+\beta} e^{-x} [\mathcal{L}_n^{(\alpha)}(x)]^2 dx \end{aligned} \quad (10)$$

(with  $x = \lambda r^2$ ,  $\alpha = l + D/2 - 1$ ,  $\beta = k/2$ ) for the radial expectation values in position space, and

$$\begin{aligned} \langle p^t \rangle &= \int p^t \gamma_{n,l,\{\mu\}}(\vec{p}) d\vec{p} = \int_0^\infty p^t \gamma_{n,l}(u) p^{D-1} dp \int |\mathcal{Y}_{l,\{\mu\}}(\Omega_D)|^2 d\Omega_D \\ &= \frac{n! \lambda^{t/2}}{\Gamma(n+l+D/2)} \int_0^\infty u^{\alpha+\epsilon} e^{-u} [\mathcal{L}_n^{(\alpha)}(u)]^2 du, \end{aligned} \quad (11)$$

(with  $u = p^2/\lambda$ ,  $\alpha = l + D/2 - 1$ , and  $\epsilon = t/2$ ) for the radial expectation values in momentum space. Note that we have taken into account the unity normalization of the hyperspherical harmonics in writing the third equality within the expressions (10) and (11). These quantities can be expressed in a closed form by means of a generalized hypergeometric function of the type  ${}_3F_2(1)$  [55] and as well they have been proved to fulfill a three-term recurrence relation [48]. These two procedures allow to find explicit expressions for a few expectation values of lowest orders [48]. However, the expression for the expectation values of higher orders is far more complicated for arbitrary states.

In this work we use a method to calculate the radial expectation values of any order for arbitrary  $D$ -dimensional harmonic states in the pseudoclassical ( $D \rightarrow \infty$ )-limit which is based on the asymptotics of power functionals of Laguerre functionals when the polynomial parameter  $\alpha \rightarrow \infty$ . This method begins with rewriting the two previous integral functionals in the form (A4) (see Corollary 1 in Appendix). Thus, we have the following expressions

$$\langle r^k \rangle = \frac{n! \lambda^{-k/2}}{\Gamma(n+l+D/2)} \int_0^\infty x^{\alpha+\sigma-1} e^{-x} [\mathcal{L}_n^{(\alpha)}(x)]^2 dx \quad (12)$$

$$\langle p^t \rangle = \frac{n! \lambda^{t/2}}{\Gamma(n+l+D/2)} \int_0^\infty u^{\alpha+\sigma-1} e^{-u} [\mathcal{L}_n^{(\alpha)}(u)]^2 du, \quad (13)$$

(with  $\sigma = \beta + 1$  and  $\sigma = \epsilon + 1$ , respect.) for the position and momentum radial expectation values, respectively. The application of this corollary to Eqs. (12) and (13) has lead us to the following ( $\alpha \rightarrow \infty$ )-asymptotics for the radial expectation values

$$\langle r^k \rangle \sim \sqrt{2\pi} \lambda^{-k/2} e^{-\alpha} \frac{\alpha^{\alpha+n+\beta+1/2}}{\Gamma(n+l+D/2)} \quad (14)$$

$$\langle p^t \rangle \sim \sqrt{2\pi} \lambda^{t/2} e^{-\alpha} \frac{\alpha^{\alpha+n+\epsilon+1/2}}{\Gamma(n+l+D/2)} \quad (15)$$

(with  $\alpha = l + D/2 - 1$ ,  $\beta = k/2$  and  $\epsilon = t/2$ ) of the harmonic states with fixed  $l$ . Now, we use the first order ( $z \rightarrow \infty$ )-asymptotic expansion of the Gamma function [77],  $\Gamma(z) \sim \sqrt{2\pi}z^{z-1/2}e^{-z}$ , and we take into account that  $(y + D)^D \sim D^D e^y$  when  $D \rightarrow \infty$ . Then, from (14) one has that the dominant term of the ( $D \rightarrow \infty$ )-asymptotics of the radial expectation values in position space is given by

$$\langle r^k \rangle \sim \left( \frac{D}{2\lambda} \right)^{\frac{k}{2}} \quad (16)$$

Note that in the large-dimensional limit the dependence on the quantum numbers is lost, what is a manifestation of the closeness to the (pseudo-) classical situation. The intrinsic quantum-mechanical structure of the system *gets hidden* in such a limit. In addition, we observe the existence of a characteristic length for this system,  $r_c = \left( \frac{D}{2\lambda} \right)^{\frac{1}{2}}$  at the pseudoclassical limit since then we have that  $\langle r \rangle \rightarrow r_c$  and  $\langle r^k \rangle \rightarrow r_c^k$ . Moreover the energy (3) can be written as  $E \rightarrow \lambda \frac{D}{2} = \lambda^2 r_c^2$ . This characteristic length corresponds to the distance at which the effective potential becomes a minimum and the ground state probability distribution has a maximum [48]. Therefore, the  $D$ -dimensional oscillator in the  $D \rightarrow \infty$  can be viewed as a particle moving in a classical orbit of radius  $r_c$  with energy  $E = \lambda^2 r_c^2$  and angular momentum  $L = \frac{D}{2}$ .

Similarly, from (15) one has the following expression for the ( $D \rightarrow \infty$ )-asymptotics of the radial expectation values in momentum space

$$\langle p^t \rangle \sim \left( \frac{\lambda D}{2} \right)^{t/2}, \quad (17)$$

so that the generalized Heisenberg-like position-momentum uncertainty product at large  $D$  is given by

$$\langle r^k \rangle \langle p^t \rangle \sim \lambda^{\frac{t-k}{2}} \left( \frac{D}{2} \right)^{\frac{k+t}{2}}. \quad (18)$$

Note that when  $k = t$  we have the Heisenberg-like uncertainty product for the large-dimensional harmonic system

$$\langle r^k \rangle \langle p^k \rangle \sim \left( \frac{D}{2} \right)^k, \quad (19)$$

which does not depend on the oscillator strength  $\lambda$ , as one would expect because of the homogenous property of the oscillator potential [79]. Thus, for  $k = 2$  we have the position-momentum uncertainty product  $\langle r^2 \rangle \langle p^2 \rangle = \frac{D^2}{4}$  in the pseudoclassical limit, which saturates not only the Heisenberg formulation of the position-momentum uncertainty principle of  $D$ -dimensional quantum physics (namely, the Heisenberg uncertainty relation  $\langle r^2 \rangle \langle p^2 \rangle \geq \frac{D^2}{4}$ ) but also the uncertainty relation for quantum systems subject to central potentials (namely,  $\langle r^2 \rangle \langle p^2 \rangle \geq \left( l + \frac{D}{2} \right)^2$ ) [80].

Finally, let us compare these  $D$ -oscillator results with the corresponding ones obtained at the pseudoclassical limit for the  $D$ -dimensional hydrogenic atom which have been recently found [58, 60]. For example, it is known that the ( $D \rightarrow \infty$ )-asymptotic second-order radial expectation values are  $\langle r^2 \rangle_H = \frac{D^4}{16Z^2}$  and  $\langle p^2 \rangle_H = \frac{4Z^2}{D^2}$  in position and momentum spaces, respectively, so that the associated Heisenberg uncertainty product is given by  $\langle r^2 \rangle_H \langle p^2 \rangle_H = \frac{D^2}{4}$ . It is most interesting to realize that the Heisenberg uncertainty product in the pseudoclassical limit has the same value for both multidimensional oscillator and hydrogenic systems, which is somehow counterintuitive taken into account that the quantum-mechanical potential is so different in the two systems.

#### IV. RÉNYI ENTROPIES OF LARGE-DIMENSIONAL HARMONIC STATES

In this section we obtain in the quasiclassical limit ( $D \rightarrow \infty$ ) the Rényi entropies of a generic  $D$ -dimensional harmonic state with the fixed hyperquantum numbers  $(n, l, \{\mu\})$  in both position and momentum spaces. Then, we express and discuss the corresponding position-momentum entropic uncertainty relation to end up with a conjecture on the Shannon-entropy-based position-momentum uncertainty relation for large-dimensional quantum systems. This might recall us some recent research on the entropic motion on curved statistical manifolds [81, 82]



We start with the expressions (8) and (9) of the position and momentum probability densities of the system, respectively. To calculate the position Rényi entropy we decompose it into two radial and angular parts. The radial part is first expressed in terms of a Rényi-like integral functional of Laguerre polynomials  $\mathcal{L}_m^{(\alpha)}(x)$  with  $\alpha = \frac{D}{2} + l - 1$ , and then this functional is determined in the large- $D$  limit by means of Theorem 1 (see Appendix A). The angular part is given by a Rényi-like integral functional of hyperspherical harmonics, which can be expressed in terms of Rényi-like functionals of Gegenbauer polynomials  $\mathcal{C}_m^{(\alpha)}$  with  $\alpha = \frac{D}{2} + l - \frac{1}{2}$ ; later on, we evaluate this Gegenbauer functional at large  $D$ , with emphasis in the circular and ( $ns$ ) states which are characterized by the hyperquantum numbers ( $n, l = n - 1, \{\mu\} = \{n - 1\}$ ) and ( $n, l = 0, \{\mu\} = \{0\}$ ), respectively.

Operating similarly in momentum space we can determine the momentum Rényi entropy of the system. In this space both the radial and angular parts of the momentum wave functions of the harmonic states are controlled by Gegenbauer polynomials as follows from the previous section.

### A. Rényi entropy in position space

Let us obtain the position Rényi entropy of the probability density  $\rho_{n,l,\{\mu\}}(\vec{r})$  given by (8), which according to (1) is defined as

$$R_q[\rho_{n,l,\{\mu\}}] = \frac{1}{1-q} \log W_q[\rho_{n,l,\{\mu\}}]; \quad 0 < q < \infty, \quad q \neq 1, \quad (20)$$

where the symbol  $W_q[\rho_{n,l,\{\mu\}}]$  denotes the entropic moments of the density

$$\begin{aligned} W_q[\rho_{n,l,\{\mu\}}] &= \int_{\mathbb{R}^D} [\rho_{n,l,\{\mu\}}(\vec{r})]^q d\vec{r} \\ &= \int_0^\infty [\rho_{n,l}(r)]^q r^{D-1} dr \times \Lambda_{l,\{\mu\}}(\Omega_{D-1}), \end{aligned} \quad (21)$$

with the angular part given by

$$\Lambda_{l,\{\mu\}}(\Omega_{D-1}) = \int_{S^{D-1}} |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^{2q} d\Omega_{D-1}. \quad (22)$$

Then, from Eqs. (21) and (20) we can obtain the total Rényi entropies of the  $D$ -dimensional harmonic state ( $n, l, \{\mu\}$ ) as follows

$$R_q[\rho_{n,l,\{\mu\}}] = R_q[\rho_{n,l}] + R_q[\mathcal{Y}_{l,\{\mu\}}], \quad (23)$$

where  $R_q[\rho_{n,l}]$  denotes the radial part

$$R_q[\rho_{n,l}] = \frac{1}{1-q} \log \int_0^\infty [\rho_{n,l}(r)]^q r^{D-1} dr, \quad (24)$$

and  $R_q[\mathcal{Y}_{l,\{\mu\}}]$  denotes the angular part

$$R_q[\mathcal{Y}_{l,\{\mu\}}] = \frac{1}{1-q} \log \Lambda_{l,\{\mu\}}(\Omega_{D-1}). \quad (25)$$

Here our aim is to determine the asymptotics of the Rényi entropy  $R_q[\rho_{n,l,\{\mu\}}]$  when  $D \rightarrow \infty$ , all the hyperquantum numbers being fixed. According to (23), this issue requires the asymptotics of the radial Rényi entropy  $R_q[\rho_{n,l}]$  and the asymptotics of the angular Rényi entropy  $R_q[\mathcal{Y}_{l,\{\mu\}}]$  given by Eqs. (24) and (25), respectively.

#### 1. Radial position Rényi entropy

From Eq. (24) the radial Rényi entropy can be expressed as

$$R_q[\rho_{n,l}] = -\log(2\lambda^{\frac{D}{2}}) + \frac{1}{1-q} \log N_{n,l}(D, q) \quad (26)$$

where  $N_{n,l}(D, q)$  denotes the following weighted-norm of the Laguerre polynomials

$$N_{n,l}(D, q) = \left( \frac{n!}{\Gamma(\alpha + n + 1)} \right)^q \int_0^\infty r^{\alpha+lq-l} e^{-qr} \left[ \mathcal{L}_n^{(\alpha)}(r) \right]^{2q} dr \tag{27}$$

with

$$\alpha = l + \frac{D}{2} - 1, \quad l = 0, 1, 2, \dots, \quad q > 0 \text{ and } \beta = (1 - q)(\alpha - l). \tag{28}$$

Note that (28) guarantees the convergence of integral functional; i.e., the condition  $\beta + q\alpha = \frac{D}{2} + lq - 1 > -1$  is always satisfied for physically meaningful values of the parameters.

Then, the determination of the asymptotics of the radial Rényi entropy  $R_q[\rho_{n,l}]$  requires the calculation of the asymptotics of the Laguerre functional  $N_{n,l}(D, q)$ ; that is, the evaluation of the Rényi-like integral functional given by (27) when  $D \rightarrow \infty$ . We do it by applying Theorem 1 (see Appendix) at zero-th order approximation to the functional  $N_{n,l}(D, q)$  given by (27) with  $(n, l)$  fixed, obtaining for every non-negative  $q \neq 1$  that

$$N_{n,l}(D, q) \sim \frac{\sqrt{2\pi}}{(n!)^q} q^{l(1-q)-1} \left( \frac{|q-1|}{q} \right)^{2qn} \frac{\alpha^{\alpha+q(l+2n)-l+\frac{1}{2}}}{[\Gamma(\alpha+n+1)]^q} (qe)^{-\alpha}, \tag{29}$$

where we have used Stirling's formula [77] for the gamma function  $\Gamma(x) = e^{-x} x^{x-\frac{1}{2}} (2\pi)^{\frac{1}{2}} [1 + \mathcal{O}(x^{-1})]$ . Then, Eqs. (26)-(29) allow us to find the following asymptotics for the radial Rényi entropy:

$$R_q[\rho_{n,l}] \sim \frac{1}{1-q} \log \left( \frac{\alpha^{\frac{D}{2}}}{\Gamma(\frac{D}{2} + n + l)^q} \right) + \frac{\frac{D}{2}}{1-q} \log \frac{\lambda^{q-1}}{qe} + \frac{q(l+2n) - \frac{1}{2}}{1-q} \log \alpha + \frac{1}{1-q} \log \mathfrak{C}(n, l, q), \tag{30}$$

(with  $\mathfrak{C}(n, l, q) = \frac{2^{q-1} \sqrt{2\pi} q^{-lq}}{(n!)^q e^{l-1}} \left( \frac{|q-1|}{q} \right)^{2qn}$ ) which can be rewritten as

$$R_q[\rho_{n,l}] \sim \frac{D}{2} \log \left( \frac{D}{2} \right) + \frac{D}{2} \log \left( \frac{q^{\frac{1}{q-1}}}{\lambda e} \right) + \left( \frac{qn}{1-q} - \frac{1}{2} \right) \log \left( \frac{D}{2} \right) + \frac{1}{1-q} \log \tilde{\mathfrak{C}}(n, l, q) \tag{31}$$

(with  $\tilde{\mathfrak{C}}(n, l, q) = \frac{e^{l-1}}{(2\pi)^{\frac{q}{2}}} \mathfrak{C}(n, l, q)$ ) or as

$$R_q[\rho_{n,l}] \sim \frac{1}{2} D \log D + \frac{1}{2} \log \left( \frac{q^{\frac{1}{q-1}}}{2\lambda e} \right) D + \left( \frac{qn}{1-q} - \frac{1}{2} \right) \log D, \tag{32}$$

which holds for  $q > 0, q \neq 1$ . Further terms in this asymptotic expansion can be obtained by means of Theorem 1. Note that, since  $q^{\frac{1}{q-1}} \rightarrow e$  when  $q \rightarrow 1$ , we have the following conjecture for the value of the radial Shannon entropy

$$\begin{aligned} S[\rho_{n,l}] &\sim \frac{D}{2} \log \left( \frac{D}{2} \right) - \frac{D}{2} \log(\lambda) \\ &= \frac{1}{2} D \log D - \frac{1}{2} D \log(2\lambda) \end{aligned} \tag{33}$$

which can be numerically shown to be correct. However a more rigorous proof for this quantity is mandatory.

Then, according to Eq. (23), to fix the asymptotics ( $D \rightarrow \infty$ ) of the total Rényi entropy  $R_q[\rho_{n,l,\{\mu\}}]$  it only remains the evaluation of the corresponding asymptotics of the angular part  $R_q[\mathcal{Y}_{l,\{\mu\}}]$  which will be done in the following.

## 2. Angular Rényi entropy

Recently it has been shown [61] that the asymptotics ( $D \rightarrow \infty$ ) of the angular part  $R_p[\mathcal{Y}_{l,\{\mu\}}]$  of the total position and momentum Rényi entropies, as defined by Eq. (25), is given by the following expression

$$\begin{aligned}
 R_q[\mathcal{Y}_{l,\{\mu\}}] &\sim \frac{1}{1-q} \log \left( \frac{\Gamma(\frac{D}{2} + l)^q}{\Gamma(\frac{D}{2} + ql)} \right) + \frac{D}{2} \log \pi \\
 &\quad + \frac{1}{1-q} \log \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \frac{\Gamma(1 + q\mu_{D-1})}{\Gamma(1 + \mu_{D-1})^q} \right) \\
 &\sim -\log \left( \Gamma \left( \frac{D}{2} \right) \right) + \frac{D}{2} \log \pi + \frac{1}{1-q} \log \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \right) \\
 &\sim -\frac{D}{2} \log \left( \frac{D}{2} \right) + \frac{D}{2} \log(e\pi) + \frac{1}{2} \log \left( \frac{D}{2} \right) + \frac{1}{1-q} \log \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \right) \\
 &\sim -\frac{1}{2} D \log D + \frac{1}{2} D \log(2e\pi) + \frac{1}{2} \log D + \frac{1}{1-q} \log \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \right)
 \end{aligned} \tag{34}$$

where

$$\tilde{\mathcal{M}}(D, q, \{\mu\}) \equiv 4^{q(l - \mu_{D-1})} \pi^{1 - \frac{D}{2}} \prod_{j=1}^{D-2} \frac{\Gamma(q(\mu_j - \mu_{j+1}) + \frac{1}{2})}{\Gamma(\mu_j - \mu_{j+1} + 1)^q} \tag{35}$$

and

$$\begin{aligned}
 \tilde{\mathcal{E}}(D, \{\mu\}) &\equiv \prod_{j=1}^{D-2} \frac{(\alpha_j + \mu_{j+1})^{2(\mu_j - \mu_{j+1})}}{(2\alpha_j + 2\mu_{j+1})_{\mu_j - \mu_{j+1}}} \frac{1}{(\alpha_j + \mu_{j+1})_{\mu_j - \mu_{j+1}}} \\
 &= \prod_{j=1}^{D-2} \frac{(\alpha_j + \mu_{j+1})^{2(\mu_j - \mu_{j+1})}}{\Gamma(2\alpha_j + \mu_{j+1} + \mu_j)} \frac{\Gamma(2\alpha_j + 2\mu_{j+1})}{\Gamma(\alpha_j + \mu_{j+1})}
 \end{aligned} \tag{36}$$

for the angular Rényi entropy of the generic harmonic state with hyperquantum numbers  $(l, \{\mu\})$ , which holds for every non-negative  $q \neq 1$ . Note that  $\tilde{\mathcal{E}} = \tilde{\mathcal{M}} = 1$  for any configuration with  $\mu_1 = \mu_2 = \dots = \mu_{D-1}$ . See Appendix B for further details.

For completeness, we will determine this asymptotic behavior in a more complete manner for some physically-relevant and experimentally accessible states like the ( $ns$ ) and circular ones, which are described by the hyperquantum numbers  $(n, l = n - 1, \{\mu\} = \{n - 1\})$  and  $(n, l = 0, \{\mu\} = \{0\})$ , respectively. Then, from Eqs. (34), (35) and (36), we have that the asymptotics of the angular part of the Rényi entropy is given by

$$R_q[\mathcal{Y}_{0,\{0\}}] \sim \log \left( \frac{2\pi^{\frac{D}{2}}}{\Gamma(\frac{D}{2})} \right) \tag{37}$$

$$\sim -\frac{D}{2} \log \left( \frac{D}{2} \right) + \frac{D}{2} \log(e\pi) + \frac{1}{2} \log \left( \frac{D}{2} \right) \tag{38}$$

$$\sim -\frac{1}{2} D \log D + \frac{1}{2} D \log(2e\pi) + \frac{1}{2} \log D \tag{39}$$

and

$$\begin{aligned}
 R_q[\mathcal{Y}_{n-1,\{n-1\}}] &\sim \frac{1}{1-q} \log \left( \left( \frac{1}{2\pi^{\frac{D}{2}}} \right)^{q-1} \frac{\left( (n)^{\frac{D}{2}-1} \right)^q}{(1+q(n-1))^{\frac{D}{2}-1}} \right) \\
 &\simeq \frac{1}{1-q} \log \left( \frac{[\Gamma(\frac{D}{2} + n - 1)]^q}{\Gamma(\frac{D}{2} + q(n-1))} \right) + \frac{D}{2} \log \pi + \frac{1}{1-q} \log \left( \frac{\Gamma(1+q(n-1))}{[\Gamma(n)]^q} \right) \\
 &\sim -\log \left( \Gamma \left( \frac{D}{2} \right) \right) + \frac{D}{2} \log \pi + \frac{1}{1-q} \log \left( \frac{\Gamma(1+q(n-1))}{[\Gamma(n)]^q} \right) \\
 &\sim \frac{D}{2} \log \frac{D}{2} + \frac{D}{2} \log(e\pi) + \frac{1}{2} \log \frac{D}{2} + \frac{1}{1-q} \log \left( \frac{\Gamma((n-1)q+1)}{\Gamma(n)^q} \right) \tag{40}
 \end{aligned}$$

$$\sim -\frac{1}{2}D \log D + \frac{1}{2}D \log(2e\pi) + \frac{1}{2} \log D + \frac{1}{1-q} \log \left( \frac{\Gamma((n-1)q+1)}{\Gamma(n)^q} \right) \tag{41}$$

for the ( $ns$ ) and circular states, respectively. Note that  $(x)_a = \frac{\Gamma(x+a)}{\Gamma(x)}$  is the well-known Pochhammer symbol [77]. Note that for very large  $D$  the dominant term of the angular Rényi entropy of these two classes of physical states is the same; namely,  $-\log \left( \Gamma \left( \frac{D}{2} \right) \right) + \frac{D}{2} \log \pi$ . Moreover and most interesting: this behavior holds for any harmonic state by taking into account in the general expression (34) that  $\tilde{\mathcal{M}}$  is dominated by factor  $\pi^{-\frac{D}{2}}$  and the growth of  $\tilde{\mathcal{E}}$  is controlled by the factor  $\frac{\Gamma(2\alpha_j+2\mu_j+1)}{\Gamma(2\alpha_j+\mu_{j+1}+\mu_j)} \frac{\Gamma(\alpha_j+\mu_j+1)}{\Gamma(\alpha_j+\mu_j)} < 1$ . Moreover, we can see in Appendix B that  $\tilde{\mathcal{M}}$  and  $\tilde{\mathcal{E}}$  are finite for fixed, finite  $l$  as it is assumed throughout the whole paper. This observation allows us to conjecture that in the limit  $q \rightarrow 1$  one has the following ( $D \rightarrow \infty$ )-asymptotics

$$\begin{aligned}
 S[\mathcal{Y}_{l,\{\mu\}}] &\sim -\log \left( \Gamma \left( \frac{D}{2} \right) \right) + \frac{D}{2} \log \pi \\
 &\sim -\frac{D}{2} \log \frac{D}{2} + \frac{D}{2} \log(e\pi) + \frac{1}{2} \log \frac{D}{2} \\
 &\sim -\frac{1}{2}D \log D + \frac{1}{2}D \log(2e\pi) + \frac{1}{2} \log D. \tag{42}
 \end{aligned}$$

for the angular Shannon entropy of the large-dimensional harmonic states.

### 3. Total position Rényi entropy

To obtain the total Rényi entropy  $R_q[\rho_{n,l,\{\mu\}}]$  in position space for a general  $(n, l, \{\mu\})$ -state, according to (23), we have to sum up the radial and angular contributions given by (32) and (34), respectively. Then, we obtain that

$$\begin{aligned}
 R_q[\rho_{n,l,\{\mu\}}] &\sim \frac{D}{2} \log \left( \frac{q^{\frac{1}{q-1}} \pi}{\lambda} \right) + \frac{qn}{1-q} \log \left( \frac{D}{2} \right) + \frac{1}{1-q} \log \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \hat{\mathcal{C}}(n, l, q) \right) \\
 &= \frac{1}{2} \log \left( \frac{q^{\frac{1}{q-1}} \pi}{\lambda} \right) D + \frac{qn}{1-q} \log D + \frac{1}{1-q} \log \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \hat{\mathcal{C}}(n, l, q) 2^{-qn} \right) \tag{43}
 \end{aligned}$$

which holds for every non-negative  $q \neq 1$  and where  $\hat{\mathcal{C}}(n, l, q) = \frac{\tilde{\mathcal{C}}(n, l, q)}{(2\pi)^{\frac{1-q}{2}}}$ . Now, for completeness and illustration we calculate this quantity in an explicit manner for the ( $ns$ ) and circular states, which both of them include the ground state. For these states we have obtained the following asymptotical expressions

$$\begin{aligned}
 R_q[\rho_{n,0,\{0\}}] &\sim \frac{D}{2} \log \left( \frac{q^{\frac{1}{q-1}} \pi}{\lambda} \right) + \frac{qn}{1-q} \log \left( \frac{D}{2} \right) + \frac{1}{1-q} \log \left( \hat{\mathcal{C}}(n, 0, q) \right) \\
 &= \frac{1}{2} \log \left( \frac{q^{\frac{1}{q-1}} \pi}{\lambda} \right) D + \frac{qn}{1-q} \log D + \frac{1}{1-q} \log \left( \hat{\mathcal{C}}(n, 0, q) 2^{-qn} \right) \tag{44}
 \end{aligned}$$

(with  $\widehat{\mathfrak{C}}(n, 0, q) = \frac{2^{q-1}}{(n!)^q} \left(\frac{|q-1|}{q}\right)^{2nq}$ ) and

$$\begin{aligned} R_q[\rho_{n,n-1,\{n-1\}}] &\sim \frac{D}{2} \log \left( \frac{q^{\frac{1}{q-1}} \pi}{\lambda} \right) + \frac{qn}{1-q} \log \left( \frac{D}{2} \right) + \frac{1}{1-q} \log \left( \widehat{\mathfrak{C}}(n, n-1, q) \right) \\ &= \frac{1}{2} \log \left( \frac{q^{\frac{1}{q-1}} \pi}{\lambda} \right) D + \frac{qn}{1-q} \log D + \frac{1}{1-q} \log \left( \widehat{\mathfrak{C}}(n, n-1, q) 2^{-qn} \right) \end{aligned} \quad (45)$$

(with  $\widehat{\mathfrak{C}}(n, n-1, q) = \frac{2^{q-1}}{(n!)^q} q^{q(1-3n)} |q-1|^{2qn}$ ), respectively. We realize from Eqs. (43), (44) and (45) that the dominant term of the  $D$ -dimensional asymptotics of the total Rényi entropy in the position space for all states  $R_q[\rho_{n,l,\{\mu\}}]$  is given by

$$R_q[\rho_{n,l,\{\mu\}}] = \frac{D}{2} \log \left( \frac{q^{\frac{1}{q-1}} \pi}{\lambda} \right) + \mathcal{O}(\log D), \quad q \neq 1 \quad (46)$$

for all fixed hyperquantum numbers. Taking into account that the ground-state Rényi entropy of the 1-dimensional harmonic oscillator is  $\frac{1}{2} \log \left( \frac{q^{\frac{1}{q-1}} \pi}{\lambda} \right)$ , this expression tells us that the dominant term corresponds to the ground-state Rényi entropy of the  $D$ -dimensional harmonic oscillator. So, the entropy variation coming from the excitation itself (which depends on the hyperquantum numbers) grows as  $\mathcal{O}(\log D)$ . To better understand this result let us keep in mind that in Cartesian coordinates the  $D$ -dimensional harmonic oscillator can be interpreted as  $D$  monodimensional oscillators; thus, for fixed  $n$  and  $D \rightarrow \infty$  we have at most a finite number of 1-dimensional modes in an excited state while an infinite number of them in the ground state.

Finally, from (46) one can conjecture that in the limit  $q \rightarrow 1$  one has

$$S[\rho_{n,l,\{\mu\}}] \sim \frac{D}{2} \log \left( \frac{e\pi}{\lambda} \right) \quad (47)$$

for the dominant term of the position Shannon entropy  $S[\rho_{n,l,\{\mu\}}]$  of a general state of the large-dimensional harmonic system with fixed hyperquantum numbers  $(n, l, \{\mu\})$ . Since the ground-state Shannon entropy of the 1-dimensional oscillator is exactly equal to  $\frac{1}{2} \log \left( \frac{e\pi}{\lambda} \right)$  [40, 50], notice that the value (47) corresponds exactly to the ground-state Shannon entropy of the  $D$ -dimensional harmonic oscillator, what it is not surprising in the light of the previous Cartesian discussion. Regrettably we cannot go further; this remains as an open problem.

## B. Rényi entropy in momentum space

The determination of the momentum Rényi entropy of a large dimensional harmonic system follows in a straightforward way from the position one because of the close relationship between the position and momentum probability densities shown in (9). Indeed one has that the momentum wave function of the system has the form

$$\tilde{\Psi}_{n,l,\{\mu\}}(\vec{p}) = \mathcal{M}_{n,l}(r) \mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}), \quad (48)$$

and the momentum density  $\gamma_{n,l,\{\mu\}}(\vec{r}) = |\tilde{\Psi}_{n,l,\{\mu\}}(\vec{p})|^2$  can be expressed as

$$\gamma_{n,l,\{\mu\}}(\vec{r}) = \gamma_{n,l}(r) |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2, \quad (49)$$

with  $\gamma_{n,l}(r) = [\mathcal{M}_{n,l}(r)]^2$ . Then, according to (9), the radial position and momentum Rényi entropies are connected as

$$R_q[\gamma_{n,l}] = R_q[\rho_{n,l}] + D \log \lambda, \quad (50)$$

which allows us to obtain the following asymptotic behavior for the radial Rényi entropy in momentum space

$$\begin{aligned} R_q[\gamma_{n,l}] &\sim \frac{D}{2} \log \left( \frac{D}{2} \right) + \frac{D}{2} \log \left( \frac{q^{\frac{1}{q-1}} \lambda}{e} \right) + \left( \frac{qn}{1-q} - \frac{1}{2} \right) \log \left( \frac{D}{2} \right) + \frac{1}{1-q} \log \tilde{\mathfrak{C}}(n, l, q) \\ &\sim \frac{1}{2} D \log D + \frac{1}{2} \log \left( \frac{q^{\frac{1}{q-1}} \lambda}{2e} \right) D + \left( \frac{qn}{1-q} - \frac{1}{2} \right) \log D. \end{aligned} \quad (51)$$

On the other hand the angular Rényi entropy  $R_p[\mathcal{Y}_{l,\{\mu\}}]$  has been previously given in Eq. (34), so that the total momentum Rényi entropy  $R_p[\gamma_{n,l,\{\mu\}}] = R_q[\gamma_{n,l}] + R_q[\mathcal{Y}_{l,\{\mu\}}]$  turns out to have the expression

$$\begin{aligned} R_q[\gamma_{n,l,\{\mu\}}] &\sim \frac{D}{2} \log \left( q^{\frac{1}{q-1}} \pi \lambda \right) + \frac{qn}{1-q} \log \left( \frac{D}{2} \right) + \frac{1}{1-q} \log \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \hat{\mathcal{C}}(n, l, q) \right) \\ &\sim \frac{1}{2} \log \left( q^{\frac{1}{q-1}} \pi \lambda \right) D + \frac{qn}{1-q} \log D + \frac{1}{1-q} \log \left( \tilde{\mathcal{E}}(D, \{\mu\})^q \tilde{\mathcal{M}}(D, q, \{\mu\}) \hat{\mathcal{C}}(n, l, q) 2^{-qn} \right). \end{aligned} \quad (52)$$

For completeness and illustration, let us give in a more complete manner the asymptotics of this quantity for some particular quantum states such as the ( $ns$ ) and circular states. For the ( $ns$ )-states we found

$$\begin{aligned} R_q[\gamma_{n,0,\{0\}}] &\sim \frac{D}{2} \log \left( q^{\frac{1}{q-1}} \pi \lambda \right) + \frac{qn}{1-q} \log \left( \frac{D}{2} \right) + \frac{1}{1-q} \log \left( \hat{\mathcal{C}}(n, 0, q) \right) \\ &= \frac{1}{2} \log \left( q^{\frac{1}{q-1}} \pi \lambda \right) D + \frac{qn}{1-q} \log D + \frac{1}{1-q} \log \left( \hat{\mathcal{C}}(n, 0, q) 2^{-qn} \right) \end{aligned} \quad (53)$$

and for the circular states we obtained the following asymptotics

$$\begin{aligned} R_q[\gamma_{n,n-1,\{n-1\}}] &\sim \frac{D}{2} \log \left( q^{\frac{1}{q-1}} \pi \lambda \right) + \frac{qn}{1-q} \log \left( \frac{D}{2} \right) + \frac{1}{1-q} \log \left( \hat{\mathcal{C}}(n, n-1, q) \right) \\ &= \frac{1}{2} \log \left( q^{\frac{1}{q-1}} \pi \lambda \right) D + \frac{qn}{1-q} \log D + \frac{1}{1-q} \log \left( \hat{\mathcal{C}}(n, n-1, q) 2^{-qn} \right). \end{aligned} \quad (54)$$

Note that for the ground state ( $n = 0$ ) one obtains that the total momentum Rényi entropy of the large-dimensional harmonic system is given by

$$R_q[\gamma_{0,0,\{0\}}] \sim \frac{D}{2} \log \left( q^{\frac{1}{q-1}} \pi \lambda \right) + \frac{1}{1-q} \log \left( \hat{\mathcal{C}}(0, 0, q) \right) \quad (55)$$

Moreover we realize that the dominant term of the total momentum Rényi entropy  $R_p[\gamma_{n,l,\{\mu\}}]$  of the large-dimensional harmonic system has the expression

$$R_q[\gamma_{n,l,\{\mu\}}] \sim \frac{D}{2} \log \left( q^{\frac{1}{q-1}} \pi \lambda \right) + \frac{qn}{1-q} \log D \quad (56)$$

Finally, from Eq. (52) one can conjecture that in the limit  $q \rightarrow 1$  one has that the Shannon entropy  $S[\gamma_{n,l,\{\mu\}}]$  in momentum space for a general ( $n, l, \{\mu\}$ )-state of the harmonic system is given by

$$S[\gamma_{n,l,\{\mu\}}] \sim \frac{D}{2} \log (e\pi\lambda). \quad (57)$$

Nevertheless it remains as an open problem a more rigorous proof of this expression because of the unknown ( $q \rightarrow 1$ )-behavior of the angular part.

### C. Position-momentum entropic uncertainty sums

From Eqs. (43) and (52) we can obtain the dominant term for the joint position-momentum Rényi uncertainty sum of a large-dimensional harmonic system. We found that for a general ( $n, l, \{\mu\}$ )-state, with  $\frac{1}{q} + \frac{1}{p} = 2$  (indeed, this relation between the parameters  $p$  and  $q$  implies that  $\frac{q}{q-1} + \frac{p}{p-1} = 0$ , which cancels the linear term in  $D$  as well as the angular factor  $\tilde{\mathcal{E}}(D, \{\mu\})$ ) gives

$$\begin{aligned} R_q[\rho_{n,l,\{\mu\}}] + R_p[\gamma_{n,l,\{\mu\}}] &\sim \frac{D}{2} \log \left( q^{\frac{1}{q-1}} p^{\frac{1}{p-1}} \pi^2 \right) \\ &\quad + \log \left( \tilde{\mathcal{M}}(D, q, \{\mu\})^{\frac{1}{1-q}} \tilde{\mathcal{M}}(D, p, \{\mu\})^{\frac{1}{1-p}} \hat{\mathcal{C}}(n, l, q) \hat{\mathcal{C}}(n, l, p) \right). \end{aligned} \quad (58)$$

For the ( $ns$ )-states the above uncertainty sum reduces to

$$R_q[\rho_{n,0,\{0\}}] + R_p[\gamma_{n,0,\{0\}}] \sim \frac{D}{2} \log \left( q^{\frac{1}{q-1}} p^{\frac{1}{p-1}} \pi^2 \right) + \log \left( \hat{\mathcal{C}}(n, 0, q) \hat{\mathcal{C}}(n, 0, p) \right), \quad (59)$$

and for the ground state as

$$R_q[\rho_{0,0,\{0\}}] + R_p[\gamma_{0,0,\{0\}}] \sim \frac{D}{2} \log \left( q^{\frac{1}{q-1}} p^{\frac{1}{p-1}} \pi^2 \right) + \log \left( \widehat{\mathcal{C}}(0,0,q) \widehat{\mathcal{C}}(0,0,p) \right). \quad (60)$$

Clearly these expressions not only fulfill the general position-momentum Rényi uncertainty relation [83–85]

$$R_q[\rho] + R_p[\gamma] \geq D \log \left( p^{\frac{1}{2(p-1)}} q^{\frac{1}{2(q-1)}} \pi \right), \quad (61)$$

but also saturate it. For the Shannon entropy, from Eqs. (47) and (57) one obtains that the leading term of the position-momentum Shannon uncertainty sum is given by

$$S[\rho_{n,l,\{\mu\}}] + S[\gamma_{n,l,\{\mu\}}] \sim D(1 + \log \pi) \quad (62)$$

which fulfills and saturates the known position-momentum Shannon uncertainty relation [86, 87]

$$S[\rho] + S[\gamma] \geq D(1 + \log \pi).$$

Finally, it is most interesting to realize that in the pseudoclassical ( $D \rightarrow \infty$ ) border the joint position-momentum Rényi-like uncertainty sum for the  $D$ -dimensional harmonic oscillator (as given by (58) has the same value as the corresponding sum for the  $D$ -dimensional hydrogenic atom which has been recently obtained [61]. This is somehow counterintuitive because of the different physico-mathematical character of the Coulomb and quadratic potential of the hydrogenic and harmonic oscillator systems, respectively.

## V. CONCLUSIONS

In this work we have determined the asymptotics ( $D \rightarrow \infty$ ) of the position and momentum Rényi and Tsallis entropies of the  $D$ -dimensional harmonic states in terms of the state's hyperquantum numbers and the harmonic parameter  $\lambda$ . We have used a recent constructive methodology which allows for the calculation of the underlying Rényi-like integral functionals of Laguerre  $\mathcal{L}_n^{(\alpha)}(x)$  and Gegenbauer  $\mathcal{C}_n^{(\alpha)}(x)$  polynomials with a fixed degree  $n$  and large values of the parameter  $\alpha$ . This is because the harmonic states are controlled by the Laguerre and Gegenbauer polynomials in both position and momentum spaces, keeping in mind that the hyperspherical harmonics (which determine the angular part of the wave functions in the two conjugated spaces) can be expressed in terms of the latter polynomials. Then, simple expressions for these quantities of some specific classes of harmonic states ( $ns$  and circular states), which include the ground state, are given.

Then, we have found the Heisenberg-like and Rényi-entropy-based equality-type uncertainty relations for all the  $D$ -dimensional harmonic oscillator states in the pseudoclassical ( $D \rightarrow \infty$ ) limit, showing that they saturate the corresponding general inequality-like uncertainty relations which are already known [80, 83–85, 91, 92]. Moreover, we have realized that these two classes of equality-type uncertainty relations which hold for the harmonic oscillator states in the pseudoclassical limit are the same as the corresponding ones for the hydrogenic atom, despite the so different mathematical character of the quantum-mechanical potential of these systems. This observation opens the way to investigate whether this property at the quantum-pseudoclassical border holds for the quantum systems with a potential other than the Coulomb and quadratic ones. In particular, does it hold for all spherically-symmetric potentials or, at least, for the potentials of the form  $r^k$  with negative or positive  $k$ ?

We should highlight that to find the Shannon entropies of the large-dimensional harmonic systems has not yet been possible with the present methodology, although the dominant term has been conjectured. A rigorous proof remains open.

Finally, let us mention that it would be very relevant for numerous quantum-mechanical systems other than the harmonic oscillator the determination of the asymptotics of integral functionals of Rényi and Shannon types for hypergeometric polynomials at large values of the polynomials' parameters and fixed degrees. Indeed, the knowledge of the asymptotics of these integral functionals would allow for the determination of the entropy and complexity measures of all quasiclassical states of the quantum systems such as e.g. the hydrogenic systems. This is yet another open problem for the future.

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**Appendix A: Rényi-like functionals of Laguerre polynomials with large parameters**

In this appendix the asymptotics ( $\alpha \rightarrow \infty$ ) of some Rényi-like functionals of Laguerre polynomials  $\mathcal{L}_n^{(\alpha)}(x)$  is given by means of the following theorem which has been recently found [88] (see also [89, 90]).

**Theorem 1.** *The Rényi-like functional of the Laguerre polynomials  $\mathcal{L}_m^{(\alpha)}(x)$  given by*

$$J_1(\sigma, \lambda, \kappa, m; \alpha) = \int_0^\infty x^{\alpha+\sigma-1} e^{-\lambda x} \left| \mathcal{L}_m^{(\alpha)}(x) \right|^\kappa dx, \tag{A1}$$

(with  $\sigma$  real,  $0 < \lambda \neq 1$ ,  $\kappa > 0$ ) has the following ( $\alpha \rightarrow \infty$ )-asymptotic behavior

$$J_1(\sigma, \lambda, \kappa, m; \alpha) \sim \alpha^{\alpha+\sigma} e^{-\alpha} \lambda^{-\alpha-\sigma-\kappa m} |\lambda - 1|^{\kappa m} \sqrt{\frac{2\pi}{\alpha}} \frac{\alpha^{\kappa m}}{(m!)^\kappa} \sum_{j=0}^\infty \frac{D_j}{\alpha^j}, \tag{A2}$$

with the first coefficients  $D_0 = 1$  and

$$D_1 = \frac{1}{12(\lambda - 1)^2} \left( 1 - 12\kappa m \sigma \lambda + 6\sigma^2 \lambda^2 - 12\sigma^2 \lambda - 6\sigma \lambda^2 + 12\sigma \lambda + 6\kappa^2 m^2 + 12\kappa m \sigma - 12\kappa m^2 \lambda - 12\kappa m \lambda + 6\kappa m \lambda^2 + 6\kappa m^2 \lambda^2 + \lambda^2 + 6\sigma^2 - 2\lambda - 6\sigma + 6\kappa m^2 \right). \tag{A3}$$

**Corollary 1.** *For the particular case  $\lambda = 1$  and  $\kappa = 2$ , i.e.,*

$$J_1(\sigma, 1, 2, m; \alpha) = \int_0^\infty x^{\alpha+\sigma-1} e^{-x} \left| \mathcal{L}_m^{(\alpha)}(x) \right|^2 dx, \tag{A4}$$

the ( $\alpha \rightarrow \infty$ )-asymptotic behavior of the integral is given by

$$I_5(m, \alpha) \sim \frac{\alpha^{\alpha+\sigma+m} e^{-\alpha}}{m!} \sqrt{\frac{2\pi}{\alpha}}. \tag{A5}$$

For the proof of Theorem 1, the knowledge of the remaining coefficients in it and other details about the theorem and the corollary, see [88].

**Appendix B: On the angular functions  $\tilde{\mathcal{E}}$  and  $\tilde{\mathcal{M}}$**

The quantum harmonic states are characterized by the hyperquantum numbers which satisfy the following restrictions:

$$\mu_1 = \dots = \mu_{k_1} > \mu_{k_1+1} = \dots = \mu_{k_2} > \mu_{k_2+1} \dots \mu_{k_i} > \mu_{k_i+1} = \dots = \mu_{k_{i+1}} > \dots \mu_{k_{N-1}} > \mu_{k_{N-1}+1} = \dots = \mu_{k_N}$$

where  $\mu_1 \equiv l$  and  $\mu_{k_N} \equiv \mu_{D-1}$ . Let us denote  $k_0 = 0$  and  $M_i$  the number of elements of the "i-th family"  $\mu_{k_{i-1}+1} = \dots = \mu_{k_i}$  so that  $\sum_{i=1}^N M_i = D - 1$ . Then we can write that

$$\begin{aligned} & \prod_{j=1}^{D-2} \frac{\Gamma(q(\mu_j - \mu_{j+1}) + \frac{1}{2})}{\Gamma(\mu_j - \mu_{j+1} + 1)^q} = \prod_{i=1}^N \left( \prod_{j=k_{i-1}+1}^{k_i-1} \frac{\Gamma(q(\mu_j - \mu_{j+1}) + \frac{1}{2})}{\Gamma(\mu_j - \mu_{j+1} + 1)^q} \right) \prod_{i=1}^{N-1} \left( \frac{\Gamma(q(\mu_{k_i} - \mu_{k_{i+1}}) + \frac{1}{2})}{\Gamma(\mu_{k_i} - \mu_{k_{i+1}} + 1)^q} \right) \\ & = \prod_{i=1}^N \left( \prod_{j=k_{i-1}+1}^{k_i-1} \Gamma\left(\frac{1}{2}\right) \right) \prod_{i=1}^{N-1} \left( \frac{\Gamma(q(\mu_{k_i} - \mu_{k_{i+1}}) + \frac{1}{2})}{\Gamma(\mu_{k_i} - \mu_{k_{i+1}} + 1)^q} \right) = \pi^{\frac{D-1-N}{2}} \prod_{i=1}^{N-1} \left( \frac{\Gamma(q(\mu_{k_i} - \mu_{k_{i+1}}) + \frac{1}{2})}{\Gamma(\mu_{k_i} - \mu_{k_{i+1}} + 1)^q} \right). \end{aligned}$$

So, the function  $\tilde{\mathcal{M}}$  defined by (35) can be expressed:

$$\begin{aligned} \tilde{\mathcal{M}}(D, q, \{\mu\}) & \equiv 4^{q(l-\mu_{D-1})} \pi^{1-\frac{D}{2}} \prod_{j=1}^{D-2} \frac{\Gamma(q(\mu_j - \mu_{j+1}) + \frac{1}{2})}{\Gamma(\mu_j - \mu_{j+1} + 1)^q} \\ & = 4^{q(l-\mu_{D-1})} \pi^{\frac{1-N}{2}} \prod_{i=1}^{N-1} \left( \frac{\Gamma(q(\mu_{k_i} - \mu_{k_{i+1}}) + \frac{1}{2})}{\Gamma(\mu_{k_i} - \mu_{k_{i+1}} + 1)^q} \right). \end{aligned}$$



In a similar way, we can express the function  $\tilde{\mathcal{E}}$  defined by (36) as:

$$\tilde{\mathcal{E}}(D, \{\mu\}) = \prod_{i=1}^{N-1} (\alpha_{k_i} + \mu_{k_{i+1}})^{2(\mu_{k_i} - \mu_{k_{i+1}})} \frac{\Gamma(2\alpha_{k_i} + 2\mu_{k_{i+1}})}{\Gamma(2\alpha_{k_i} + \mu_{k_i} + \mu_{k_{i+1}})} \frac{\Gamma(\alpha_{k_i} + \mu_{k_{i+1}})}{\Gamma(\alpha_{k_i} + \mu_{k_i})} \sim \left(\frac{1}{2}\right)^{(l - \mu_{D-1})}.$$

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### 3.3 General stationary states

In this section we extend the research done in the two previous sections about the Rényi entropies for the Rydberg and pseudo-classical states of the multidimensional harmonic system in the following sense: here we obtain the Rényi entropies with a natural parameter for all ground and excited stationary states of the multidimensional harmonic system. Then, we also determine their associated uncertainty relations in terms of the basic parameters which characterize the system. These aims have been obtained by means of the linearization methods of hypergeometric orthogonal polynomials described in Section 1.3 together with the algebraic properties of the Laguerre and Gegenbauer polynomials and other special functions of Applied Mathematics and Mathematical Physics [59].

Summarizing, the following tasks have been achieved:

- Calculation of the Rényi entropies with a natural parameter  $q$  for all discrete stationary states of the multidimensional harmonic system in terms of the Rényi index  $q$ , the spatial dimensionality and the oscillator strength, as well as the hyperquantum numbers,  $\{n_i\}_{i=1}^D$ , associated to the Cartesian coordinates of the system, which characterize the corresponding state's wavefunction. The final expressions with positive integer index  $q$  in both position and momentum spaces are given by means of the generalized Lauricella hypergeometric functions of type A.
- Determination of the associated entropic uncertainty sums, showing the saturation of the general entropic uncertainty relations of Bialynicki-Birula [91] and Zozor-Vignat [92, 93].

It remains as an open problem, the extension of this result to Rényi entropies for any real value of the parameter  $q$ . The latter requires, however, an approach other than that based on the use of Cartesian coordinates and the linearization methodology used here. Such an approach is still unknown to the best of our knowledge.

These results have been published in the article [66] with coordinates: **Puertas-Centeno D.**, Toranzo, I.V. and Dehesa J.S. *Exact Rényi entropies of D-dimensional harmonic systems*. European Physical Journal-Special Topics, 2018 (accepted), which is attached below.

# Exact Rényi entropies of $D$ -dimensional harmonic systems

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The determination of the uncertainty measures of multidimensional quantum systems is a relevant issue *per se* and because these measures, which are functionals of the single-particle probability density of the systems, describe numerous fundamental and experimentally accessible physical quantities. However, it is a formidable task (not yet solved, except possibly for the ground and a few lowest-lying energetic states) even for the small bunch of elementary quantum potentials which are used to approximate the mean-field potential of the physical systems. Recently, the dominant term of the Heisenberg and Rényi measures of the multi-dimensional harmonic system (i.e., a particle moving under the action of a  $D$ -dimensional quadratic potential,  $D > 1$ ) has been analytically calculated in the high-energy (i.e., Rydberg) and the high-dimensional (i.e., pseudoclassical) limits. In this work we determine the exact values of the Rényi uncertainty measures of the  $D$ -dimensional harmonic system for all ground and excited quantum states directly in terms of  $D$ , the potential strength and the hyperquantum numbers.

## I. INTRODUCTION

The Rényi entropy of the probability density  $\rho(\vec{r})$ ,  $\vec{r} = (x_1, \dots, x_D)$ , which characterizes the quantum state of a  $D$ -dimensional physical system is defined [1, 2] as

$$R_q[\rho] = \frac{1}{1-q} \log W_q[\rho], \quad 0 < q < \infty, \quad q \neq 1, \quad (1)$$

where the symbol  $W_q[\rho]$  denotes the frequency or entropic moment of order  $q$  of the density given by

$$W_q[\rho] = \int_{\mathbb{R}^D} [\rho(\vec{r})]^q d\vec{r}. \quad (2)$$

These quantities completely characterize the density  $\rho(\vec{r})$  [3, 4] under certain conditions. They quantify numerous facets of the spreading of the quantum probability density  $\rho(\vec{r})$ , which include

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the intrinsic randomness (uncertainty) and the geometrical profile of the quantum system. The Rényi entropies are closely related to the Tsallis entropies [8]  $T_p[\rho] = \frac{1}{p-1}(1 - W_p[\rho])$ ,  $0 < p < \infty$ ,  $p \neq 1$  by  $T_p[\rho] = \frac{1}{1-p}[e^{(1-p)R_p[\rho]} - 1]$ . Moreover for the special cases  $q = 0, 1, 2$ , and  $\infty$ , the Rényi entropic power,  $N_q[\rho] = e^{R_q[\rho]}$ , is equal to the length of the support,  $e^{-\langle \ln \rho \rangle}$ ,  $\langle \rho \rangle^{-1}$ ,  $\rho_{max}^{-1}$ , respectively. Therefore, these  $q$ -entropies include the Shannon entropy [7],  $S[\rho] = \lim_{p \rightarrow 1} R_p[\rho] = \lim_{p \rightarrow 1} T_p[\rho]$ , and the disequilibrium,  $\langle \rho \rangle = \exp(-R_2[\rho])$ , as two important particular cases; in addition, they The use of Rényi, Shannon and Tsallis entropies as measures of uncertainty allow a wider quantitative range of applicability than the Heisenberg-like measures which are based on the moments around the origin (so, including the standard or root-square-mean deviation). This permits, for example, a quantitative discussion of quantum uncertainty relations further beyond the conventional Heisenberg-like uncertainty relations [9–15]. The properties of the Rényi entropies and their applications have been widely analyzed; see e.g. [16–18] and the reviews [9, 19, 20].

In general, the Rényi entropies of quantum systems cannot be determined in an exact way, basically because the associated wave equation is generally not solvable in an analytical way. Even when the time-independent Schrödinger equation is solvable, what happens for a small set of elementary potentials (zero-range, harmonic, Coulomb) [21, 22], the exact determination of the Rényi entropies is a formidable task mainly because they are integral functionals of some special functions of applied mathematics [23] (e.g., orthogonal polynomials, hypergeometric functions, Bessel functions,...) which control the wavefunctions of the stationary states of the quantum system. These integral functionals have not yet been solved for harmonic (i.e., oscillator-like) systems except for a few lowest-lying states (where the calculation is trivial) and, most recently, for the extreme Rydberg (i.e., highest-lying) [24–26] and pseudoclassical (i.e., the highest dimensional) [15, 27, 28] states of harmonic and Coulomb systems by means of sophisticated asymptotical techniques of orthogonal polynomials. This lack is amazing because harmonicity is the most frequent and useful approximation to study the quantum many-body systems, and the other two basic classes of uncertainty measures, the Heisenberg-like measures [29–36] and the Fisher information [37], have been already calculated for all stationary states of the multidimensional harmonic system.

In this work we determine the exact values of the Rényi uncertainty measures of the  $D$ -dimensional harmonic system (i.e., a particle moving under the action of a quadratic potential) for all ground and excited quantum states directly in terms of  $D$ , the potential strength and the hyperquantum numbers which characterize the states. This is a far more difficult problem than the Heisenberg-like and Fisher information cases, both analytically and numerically. The latter

is basically because a naive numerical evaluation using quadratures is not convenient due to the increasing number of integrable singularities when the principal hyperquantum number is increasing, which spoils any attempt to achieve reasonable accuracy even for rather small hyperquantum numbers [38].

The structure of the manuscript is the following. In section II the wavefunctions and the probability densities of the stationary states of the  $D$ -dimensional harmonic (oscillator-like) system are briefly described in both position and momentum spaces. In section III the Rényi entropies for all the ground and excited states of this system are determined in an analytical way by use of a recently developed methodology [39]. Finally some conclusions and open problems are given.

## II. THE $D$ -DIMENSIONAL HARMONIC PROBLEM

In this section we summarize the quantum-mechanical  $D$ -dimensional problem corresponding to the harmonic oscillator potential

$$V(r) = \frac{1}{2}k(x_1^2 + \dots + x_D^2) = \frac{1}{2}kr^2, \quad (3)$$

and we give the probability densities of the stationary quantum states of the system in both position and momentum spaces. The stationary bound states of the system, which are the physical solutions of the Schrödinger equation

$$\left(-\frac{1}{2}\vec{\nabla}_D^2 + V(r)\right)\Psi(\vec{r}) = E\Psi(\vec{r}), \quad (4)$$

(we use atomic units throughout the paper) where  $\vec{\nabla}_D$  denotes the  $D$ -dimensional gradient operator, are well known [40–42] to be characterized by the energies

$$E_N = \left(N + \frac{D}{2}\right)\omega \quad (5)$$

where

$$\omega = \sqrt{k}, \quad N = \sum_{i=1}^D n_i \quad \text{with} \quad n_i = 0, 1, 2, \dots$$

The corresponding eigenfunctions can be expressed as

$$\psi_N(\vec{r}) = \mathcal{N}e^{-\frac{1}{2}\alpha(x_1^2 + \dots + x_D^2)} H_{n_1}(\sqrt{\alpha}x_1) \cdots H_{n_D}(\sqrt{\alpha}x_D), \quad \alpha = k^{\frac{1}{4}} \quad (6)$$

where  $\vec{r} \in \mathbb{R}^D$  and  $\mathcal{N}$  stands for the normalization constant

$$\mathcal{N} = \frac{1}{\sqrt{2^N n_1! n_2! \cdots n_D!}} \left(\frac{\alpha}{\pi}\right)^{D/4},$$



and  $H_n(x)$  denotes the Hermite polynomials of degree  $n$  orthogonal with respect the weight function  $\omega(x) = e^{-x^2}$  in  $(-\infty, \infty)$ .

Then, the associated quantum probability density in position space is given by

$$\rho_N(\vec{r}) = |\psi_N(\vec{r})|^2 = \mathcal{N}^2 e^{-\alpha(x_1^2 + \dots + x_D^2)} H_{n_1}^2(\sqrt{\alpha} x_1) \cdots H_{n_D}^2(\sqrt{\alpha} x_D), \quad (7)$$

and the density function in momentum space is obtained by squaring the Fourier transform of the position wavefunction, obtaining

$$\gamma_N(\vec{p}) = \tilde{\mathcal{N}}^2 e^{-\frac{1}{\alpha}(p_1^2 + \dots + p_D^2)} H_{n_1}^2\left(\frac{p_1}{\sqrt{\alpha}}\right) \cdots H_{n_D}^2\left(\frac{p_D}{\sqrt{\alpha}}\right) = \alpha^{-D} \rho_N\left(\frac{\vec{p}}{\alpha}\right) \quad (8)$$

where  $\vec{p} \in \mathbb{R}^D$  and the normalization constant is

$$\tilde{\mathcal{N}} = \frac{1}{\sqrt{2^N n_1! \cdots n_D!}} \left(\frac{1}{\pi\alpha}\right)^{D/4}.$$

### III. RÉNYI ENTROPIES OF THE HARMONIC SYSTEM

Let us now determine the Rényi entropy of the  $D$ -dimensional harmonic system according to Eqs. (1)-(2) by

$$\begin{aligned} R_q[\rho_N] &= \frac{1}{1-q} \log \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_D [\rho_N(\vec{r})]^q \\ &= \frac{1}{1-q} \log \left( \mathcal{N}^{2q} \int_{-\infty}^{\infty} e^{-\alpha q x_1^2} |H_{n_1}(\sqrt{\alpha} x_1)|^{2q} dx_1 \cdots \int_{-\infty}^{\infty} e^{-\alpha q x_D^2} |H_{n_D}(\sqrt{\alpha} x_D)|^{2q} dx_D \right) \end{aligned} \quad (9)$$

where we have used Eq. (7). To calculate these  $D$  integral functionals of Hermite polynomials we will follow the 2013-dated technique (only valid for  $q \in \mathbb{N}$  other than unity) [5, 6, 39] to evaluate similar integral functionals of hypergeometric orthogonal polynomials by means of multivariate special functions. To do so, first we express the Hermite polynomials in terms of the Laguerre polynomials (see e.g., [43]) as

$$\begin{aligned} H_{2n}(x) &= (-1)^n 2^{2n} n! L_n^{-\frac{1}{2}}(x^2), \\ H_{2n+1}(x) &= (-1)^n 2^{2n+1} n! x L_n^{\frac{1}{2}}(x^2), \end{aligned} \quad (10)$$

which allows to write

$$H_n(\sqrt{\alpha} x)^{2q} = A_{n,q}(\nu) \alpha^{q\nu} x^{2q\nu} L_{\frac{n-\nu}{2}}^{(\nu-\frac{1}{2})}(\alpha x^2)^{2q}, \quad (11)$$

with the constant

$$A_{n,q}(\nu) = 2^{2qn} \left[ \Gamma \left( \frac{n-\nu}{2} + 1 \right) \right]^{2q}$$

and the parameter  $\nu = 0(1)$  for even(odd)  $n$ ; that is,  $\nu = \frac{1}{2}(1 - (-1)^n)$ .

Following the same steps as in [39], after the change of variable  $t_i = \alpha q x_i^2$  in (9), one obtains the following linearization relation for the  $(2q)$ -th power of the Hermite polynomials

$$H_n(\sqrt{\alpha}x)^{2q} = A_{n,q}(\nu)q^{-q\nu} \sum_{j=0}^{\infty} \frac{1}{(-1)^{2^j} j!} c_j \left( q\nu, 2q, \frac{1}{q}, \frac{n-\nu}{2}, \nu - \frac{1}{2}, -\frac{1}{2} \right) H_{2j}(\sqrt{\alpha}qx), \quad (12)$$

with

$$\begin{aligned} c_j \left( q\nu, 2q, \frac{1}{q}, \frac{n-\nu}{2}, \nu - \frac{1}{2}, -\frac{1}{2} \right) &= \\ &= \left( \frac{1}{2} \right)_{q\nu} \left( \frac{n+\nu-1}{2} \right)_{2q} F_A^{(2q+1)} \left( \begin{matrix} q\nu + \frac{1}{2}; \overbrace{\frac{\nu-n}{2}, \dots, \frac{\nu-n}{2}}^{2q}, -j \\ \underbrace{\nu + \frac{1}{2}, \dots, \nu + \frac{1}{2}}_{2q}, \frac{1}{2} \end{matrix} ; \underbrace{\frac{1}{q}, \dots, \frac{1}{q}}_{2q}, 1 \right), \end{aligned} \quad (13)$$

where  $(z)_a = \frac{\Gamma(z+a)}{\Gamma(z)}$  is the known Pochhammer's symbol and  $F_A^{(2q+1)}(\frac{1}{q}, \dots, \frac{1}{q}, 1)$  is the Lauricella function of type A of  $2q+1$  variables given by

$$\begin{aligned} F_A^{(2q+1)} \left( \begin{matrix} q\nu + \frac{1}{2}; \frac{\nu-n}{2}, \dots, \frac{\nu-n}{2}, -j \\ \nu + \frac{1}{2}, \dots, \nu + \frac{1}{2}, \frac{1}{2} \end{matrix} ; \frac{1}{q}, \dots, \frac{1}{q}, 1 \right) &= \\ &= \sum_{k_1, \dots, k_{2q}, k_{2q+1}=0}^{\infty} \frac{\left( q\nu + \frac{1}{2} \right)_{k_1 + \dots + k_{2q} + k_{2q+1}} \left( \frac{\nu-n}{2} \right)_{k_1} \dots \left( \frac{\nu-n}{2} \right)_{k_{2q}} (-j)_{k_{2q+1}} \left( \frac{1}{q} \right)^{k_1} \dots \left( \frac{1}{q} \right)^{k_{2q}}}{\left( \nu + \frac{1}{2} \right)_{k_1} \dots \left( \nu + \frac{1}{2} \right)_{k_{2q}} \left( \frac{1}{2} \right)_{k_{2q+1}}} \frac{1}{k_1! \dots k_{2q}! k_{2q+1}!}, \end{aligned} \quad (14)$$

Now, the combination of Eqs. (9) and (12) together with the orthogonalization condition of the Hermite polynomials  $H_n(x)$  (with which one realizes that all the summation terms vanish except

the one with  $i = 0$ ), allows one to write the exact Rényi entropy of the harmonic system as

$$\begin{aligned} R_q[\rho_N] &= \frac{1}{1-q} \log \left[ \mathcal{N}^{2q} \left( \frac{\pi}{\alpha} \right)^{\frac{D}{2}} q^{-\frac{D}{2}} \prod_{i=1}^D q^{-q\nu_i} A_{n_i, q}(\nu_i) c_0 \left( q\nu_i, 2q, \frac{1}{q}, \frac{n_i - \nu_i}{2}, \nu_i - \frac{1}{2}, -\frac{1}{2} \right) \right] \\ &= \frac{D}{2} \log \left[ \frac{\pi}{\alpha} \right] + \frac{1}{q-1} \log \left[ 2^{qN} q^{\frac{D}{2}} \right] + \frac{1}{1-q} \sum_{i=1}^D \log \left[ \frac{A_{n_i, q}(\nu_i)}{q^{q\nu_i} \Gamma(n_i + 1)^q} c_0 \left( q\nu_i, 2q, \frac{1}{q}, \frac{n_i - \nu_i}{2}, \nu_i - \frac{1}{2}, -\frac{1}{2} \right) \right] \end{aligned} \quad (15)$$

with

$$c_0 \left( q\nu, 2q, \frac{1}{q}, \frac{n - \nu}{2}, \nu - \frac{1}{2}, -\frac{1}{2} \right) = \left( \frac{1}{2} \right)_{q\nu} \left( \frac{\frac{n+\nu-1}{2}}{\frac{n-\nu}{2}} \right)^{2q} \mathfrak{F}_q(n), \quad (16)$$

where the symbol  $\mathfrak{F}_q(n)$  denotes the following Lauricella function of  $2q$  variables

$$\begin{aligned} \mathfrak{F}_q(n) &\equiv F_A^{(2q+1)} \left( \begin{matrix} q\nu + \frac{1}{2}; \frac{\nu-n}{2}, \dots, \frac{\nu-n}{2}, 0 \\ \nu + \frac{1}{2}, \dots, \nu + \frac{1}{2}, \frac{1}{2} \end{matrix} ; \frac{1}{q}, \dots, \frac{1}{q}, 1 \right) = F_A^{(2q)} \left( \begin{matrix} q\nu + \frac{1}{2}; \frac{\nu-n}{2}, \dots, \frac{\nu-n}{2} \\ \nu + \frac{1}{2}, \dots, \nu + \frac{1}{2} \end{matrix} ; \frac{1}{q}, \dots, \frac{1}{q} \right) \\ &= \sum_{j_1, \dots, j_{2q}=0}^{\infty} \frac{(q\nu + \frac{1}{2})_{j_1 + \dots + j_{2q}} (\frac{\nu-n}{2})_{j_1} \dots (\frac{\nu-n}{2})_{j_{2q}} \left( \frac{1}{q} \right)^{j_1} \dots \left( \frac{1}{q} \right)^{j_{2q}}}{(\nu + \frac{1}{2})_{j_1} \dots (\nu + \frac{1}{2})_{j_{2q}} j_1! \dots j_{2q}!} \\ &= \sum_{j_1, \dots, j_{2q}=0}^{\frac{n-\nu}{2}} \frac{(q\nu + \frac{1}{2})_{j_1 + \dots + j_{2q}} (\frac{\nu-n}{2})_{j_1} \dots (\frac{\nu-n}{2})_{j_{2q}} \left( \frac{1}{q} \right)^{j_1} \dots \left( \frac{1}{q} \right)^{j_{2q}}}{(\nu + \frac{1}{2})_{j_1} \dots (\nu + \frac{1}{2})_{j_{2q}} j_1! \dots j_{2q}!}. \end{aligned} \quad (17)$$

Note that, as  $\frac{\nu-n}{2}$  is always a negative integer number, the Lauricella function simplifies to a finite sum. In the following, for convenience, we use the notation  $N_O = \sum_{i=1}^D \nu_i$ , which is the amount of odd numbers  $n_i$  and, thus,  $N_E = D - N_O$  gives the number of the even ones. Then simple algebraic manipulations allow us to rewrite Eq. (15) as

$$R_q[\rho_N] = -\frac{D}{2} \log[\alpha] + \mathcal{K}_q D + \bar{\mathcal{K}}_q N_O + \frac{q}{q-1} \sum_{i=1}^D (-1)^{n_i} \log \left[ \left( \frac{n_i + 1}{2} \right)_{\frac{1}{2}} \right] + \frac{1}{1-q} \sum_{i=1}^D \log[\mathfrak{F}_q(n_i)], \quad (18)$$

where  $\mathcal{K}_q = \frac{\log[\pi^{q-\frac{1}{2}} q^{\frac{1}{2}}]}{q-1}$  and  $\bar{\mathcal{K}}_q = \frac{1}{1-q} \log \left[ \frac{4^q \Gamma(\frac{1}{2}+q)}{\pi^{\frac{1}{2}} q^q} \right]$ . This expression allows for the analytical determination of the Rényi entropies (with positive integer values of  $q$ ) for any arbitrary state of the multidimensional harmonic systems.

Finally, for the ground state (i.e.,  $n_i = 0, i = 1, \dots, D$ ; so,  $N = 0$ ) the general Eq. (18) boils down to ,

$$R_q[\rho_N] = \frac{D}{2} \log \left[ \frac{\pi q^{\frac{1}{q-1}}}{\alpha} \right]. \quad (19)$$

In fact, this ground state Rényi entropy holds for any  $q > 0$  as one can directly derive from Eq. (9). Taking into account that the momentum density is a re-scaled form of the position density, we have the following expression for the associated momentum Rényi entropy,

$$R_{\tilde{q}}[\gamma_N] = \frac{D}{2} \log [\alpha] + \mathcal{K}_{\tilde{q}} D + \bar{\mathcal{K}}_{\tilde{q}} N_O + \frac{\tilde{q}}{\tilde{q}-1} \sum_{i=1}^D (-1)^{n_i} \log \left[ \left( \frac{n_i+1}{2} \right)_{\frac{1}{2}} \right] + \frac{1}{1-\tilde{q}} \sum_{i=1}^D \log [\mathfrak{F}_{\tilde{q}}(n_i)], \quad (20)$$

( $\tilde{q} \in \mathbb{N}$ ). Although Eqs. (18) and (20) rigorously hold for  $q \neq 1$  and  $q \in \mathbb{N}$  only, it seems reasonable to conjecture its general validity for any  $q > 0, q \neq 1$  provided the formal existence of a generalized function  $\mathfrak{F}_q(n)$ . If so, we obtain the general expression for the position-momentum uncertainty Rényi entropic sum as

$$R_q[\rho_N] + R_{\tilde{q}}[\gamma_N] = (\mathcal{K}_q + \mathcal{K}_{\tilde{q}}) D + (\bar{\mathcal{K}}_q + \bar{\mathcal{K}}_{\tilde{q}}) N_O + \left( \frac{q}{q-1} + \frac{\tilde{q}}{\tilde{q}-1} \right) \sum_{i=1}^D (-1)^{n_i} \log \left[ \left( \frac{n_i+1}{2} \right)_{\frac{1}{2}} \right] + \frac{1}{1-q} \sum_{i=1}^D \log [\mathfrak{F}_q(n_i)] + \frac{1}{1-\tilde{q}} \sum_{i=1}^D \log [\mathfrak{F}_{\tilde{q}}(n_i)] \quad (21)$$

which verifies the Rényi-entropy-based uncertainty relation of Zozor-Portesi-Vignat [13] when  $\frac{1}{q} + \frac{1}{\tilde{q}} \geq 2$  for arbitrary quantum systems. In the conjugated case  $\tilde{q} = q^*$  such that  $\frac{1}{q} + \frac{1}{q^*} = 2$ , one obtains

$$R_q[\rho_N] + R_{q^*}[\gamma_N] = D \log \left( \pi q^{\frac{1}{2q-2}} q^{*\frac{1}{2q^*-2}} \right) + (\bar{\mathcal{K}}_q + \bar{\mathcal{K}}_{q^*}) N_O + \frac{1}{1-q} \sum_{i=1}^D \log [\mathfrak{F}_q(n_i)] + \frac{1}{1-q^*} \sum_{i=1}^D \log [\mathfrak{F}_{q^*}(n_i)]. \quad (22)$$

Let us finally remark that the first term corresponds to the sharp bound for the general Rényi entropy uncertainty relation with conjugated parameters

$$R_q[\rho_N] + R_{q^*}[\gamma_N] \geq D \log \left( \pi q^{\frac{1}{2q-2}} q^{*\frac{1}{2q^*-2}} \right)$$

of Bialynicki-Birula [11] and Zozor-Vignat [12].

#### IV. CONCLUSIONS

In this work we have explicitly calculated the Rényi entropies,  $R_q[\rho_N]$  ( $q \in \mathbb{N}$ ), for all the quantum-mechanically allowed harmonic states in terms of the Rényi index  $q$ , the spatial dimension  $D$ , the oscillator strength  $\alpha$ , as well as the hyperquantum numbers,  $\{n_i\}_{i=1}^D$ , which characterize the corresponding state's wavefunction. To do that we have used the harmonic wavefunctions in Cartesian coordinates, which can be expressed in terms of a product of  $D$  Hermite polynomials and exponentials. So, the Rényi entropies of the quantum states boil down to  $D$  entropy-like functionals of Hermite polynomials. Then we have determined these integral functionals by taking into account the close connection between the Hermite and Laguerre polynomials and the Srivastava-Niukkanen linearization method for powers of Laguerre polynomials. The final analytical expression of the Rényi entropies with positive integer index  $q$  in both position and momentum spaces is given in a compact way by use of a Lauricella function of type A. It remains as an open problem, the extension of this result to Rényi entropies for any real value of the parameter  $q$ . The latter requires a completely different approach, still unknown to the best of our knowledge.

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## Part II

# Complexity of multidimensional quantum phenomena



# Introduction

Complexity of a finite many-particle system is a primary notion of the same character as e.g., energy and information. Perhaps this is because it has too many facets to be captured by a single quantifier. Nowadays, a systematic treatment of the intuitive idea of complexity is unknown despite the great efforts done in many areas of science and technology from atomic, molecular and nuclear physics up to the adaptive complex systems and ultimately the living beings [1, 2, 38, 40, 203–208].

The quantum many-particle systems are intrinsically complex in ways that are fundamentally different from any product of design. The quantification of complexity attributed to many-particle systems, which is closely connected with evolution from order to disorder, is among the most important scientific challenges in the theory of complex systems [1, 39, 40]. Intuitively, the complexity of a finite many-particle system is a measure of the internal order/disorder of the system in question, which must be closely connected with the notion of information and its main quantifier, the information entropy. Interpreting the second law of thermodynamics, which indicates an always increasing entropy, one can vaguely explain the fact that information entropy is maximal for a completely disordered system. Presently, however, there is no universal law which governs the complexity of the physical systems. A completely ordered or completely regular system (e.g., a perfect crystal) is obviously non-complex, but also the structure of a completely disordered or absolutely random system (e.g, an ideal gas) enjoys a very simple description. We say that these two extremal cases have no complexity, or rather an extremely low, minimum complexity.

To formalize the intuitive notion of complexity of a physical system in a physico-mathematical way, various theoretico-informational quantities have been proposed. They can be classified in two broad groups: the intrinsic complexity measures (which only depend on the single-particle probability distribution of the system) [1, 7, 204–206, 208] and the Kolmogorov-like or extrinsic complexity measures [2, 38, 40, 203, 209]. The latter ones, also called algorithmic complexity measures, are based on the idea that complexity can be quantify through the complexity of its simplest mathematical model; that is, the model which requires the minimal information of the past to be able to predict the optimal behavior of the system for the future.

Part II is centered around the intrinsic complexity measures, since we are interested in the internal disorder of the quantum complex systems (i.e., the structure, organization and correlation of their elementary constituents). Among the numerous statistical quantifiers of this type which have been studied in the last two decades [38, 54, 113, 203–205, 208, 210–231, 231–251], let us highlight the two-factor complexity measures which are very relevant in numerous scientific and technological fields. They are given by the product of two dispersion/entropic measures appropriately renormalized in order to have a number of relevant properties such as the invariance under replication, translation and scaling transformations and the monotonicity with respect to a class of operations [252]. The most familiar two-factor complexity measures are the Crámer-Rao, Fisher-Shannon and LMC (López-ruiz-Mancini-Calvet) complexities and its generalizations, the Fisher-Rényi and LMC-Rényi complexities.

**The goal of Part II** is to extend these basic two-factor complexity measures (i) by generating novel families of bi- and tri-parametric complexity quantifiers and by studying their fundamental properties. Moreover, these multiparametric complexity measures are shown to be very useful by applying them to some multidimensional quantum systems and phenomena such as the generalized Planck distribution and the harmonic and hydrogenic systems. This has been done by means of (i) the ideas and techniques of Lutwak [119, 121] and Bercher [120], which extend the Crámer-Rao and Stam inequalities to a  $q$ -Gaussian context by using a biparametric version of the Fisher information, and (ii) the novel notion of differential-escort transformation [71], which has allowed us to prove the monotonicity of the LMC-Rényi complexity measure as well as to extend the biparametric Stam inequality to a tri-parametric one, and exactly compute the optimal bound and the explicit expression for the minimizing densities (which extend the  $q$ -Gaussian densities).

The structure of Part II is composed by four chapters. Chapter 4 contains a brief review of the basic two-factor complexity measures used in this work together with their main inequality-type properties. In Chapter 5 we introduce the notions of the biparametric complexity measures of Fisher-Rényi and Crámer-Rao types, we discuss their properties and we apply them to the frequency spectrum of the blackbody radiation at a given temperature in universes with standard and non-standard dimensionalities. In Chapter 6 the notion of differential-escort transformation is defined and discussed. We illustrate its utility by proving the monotonicity property of the LMC-Rényi complexity measure with respect to differential-escort transformations. Then, the entropic properties of the differential-escort distributions for a general probability density are shown, and the extreme low and high complexity limits are carefully studied. Moreover, the Tsallis  $q$ -exponential densities are shown to correspond to the differential-escort transformations of the exponential one. Finally, in Chapter 7 we generalize the Stam inequality until to a triparametric one for univariate probability distributions, we compute analytically the exact bound and moreover, we give the family of the associated minimizer probability

densities. The resulting triparametric Stam inequality and the generated triparametric Fisher-Rényi are then applied to the radial density of the hydrogenic and harmonic systems.

## Chapter 4

# Complexity measures and inequality-type properties

The physical and chemical properties of the multidimensional quantum many-particle systems are controlled [6] by means of the spatial delocalization or spreading of the single-particle density  $\rho(\vec{r})$ ,  $\vec{r} \in \Delta \subseteq \mathbb{R}_d$  defined as

$$\rho(\vec{r}) := \sum_{\sigma_1, \sigma_2, \dots, \sigma_n} \int_{\Delta} |\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n; \sigma_1, \sigma_2, \dots, \sigma_n)|^2 d\vec{r}_2 \dots d\vec{r}_n \quad (4.1)$$

where  $\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n; \sigma_1, \sigma_2, \dots, \sigma_n)$  represents the wave function of the  $d$ -dimensional  $n$ -particle system, and  $\vec{r} = (x_1, x_2, \dots, x_d)$ ,  $\sigma_i \in (-\frac{1}{2}, \frac{1}{2})$ , and  $(r_i, \sigma_i)$  denote the position-spin coordinates of the  $i$ th-particle, which is assumed to be normalized and antisymmetrized in the pairs  $(\vec{r}_i, \sigma_i)$ .

In this chapter we briefly review the basic complexity measures of Crámer-Rao, Fisher-Shannon and LMC types of a multidimensional probability distribution  $\rho(\vec{r})$ ,  $\vec{r} \in \Delta \subseteq \mathbb{R}_d$ , and their generalizations (Fisher-Rényi, LMC-Rényi) together with their inequality-type properties. They have been used to investigate of a great deal of physical phenomena of numerous finite quantum many-body systems [1, 229, 238–242, 253].

These three complexity measures (Crámer-Rao, Fisher-Shannon, LMC) are known to be dimensionless, invariant under translation and scaling transformation [205, 207], and universally bounded from below by unity [7, 109, 175, 244]. The question whether these quantities are minimum for the two extreme (or *least complex*) distributions corresponding to perfect order and maximum disorder (associated to an extremely localized Dirac delta distribution and a highly flat distribution in the one dimensional case, respectively) is a long standing and controverted issue [135, 204, 252] which has been partially solved. The Crámer-Rao and Fisher-Shannon measures have been recently shown to be monotone in a well-defined sense [252], contrary the LMC measure. Here the monotonicity problem of the LMC measure is examined.

## 4.1 Measures of Crámer-Rao type

The Crámer-Rao measure of complexity, inspired by the Crámer-Rao inequality [254, 255], is defined [241, 243, 256] by the product of the variance  $V[\rho]$  and the Fisher information  $F[\rho]$  as

$$C^{(CR)}[\rho] := F[\rho] \times V[\rho], \quad (4.2)$$

which is composed by a local ingredient, the Fisher information, and a global one, the variance. So, this quantity measures the gradient content of the density jointly with the concentration of the probability cloud around the centroid. Assuming that  $|\langle \vec{r} \rangle|^2 = 0$ , what rigorously holds for systems with a spherically-symmetric quantum-mechanical potential, one has that the Crámer-Rao complexity measure fulfills

$$C_{CR}[\rho] = F[\rho] \times \langle r^2 \rangle \geq d^2, \quad (4.3)$$

which holds for all the stationary bound states of the  $D$ -dimensional quantum systems [30, 108, 109]. It is known that the lower bound  $D^2$  is reached by the (Gaussian) density associated with the ground state of the harmonic oscillator in an unbounded domain  $\Delta$ ; see [29, 108, 257] for further details. Moreover, the Crámer-Rao complexity is related to the Heisenberg uncertainty product  $\langle r^2 \rangle \langle p^2 \rangle$  as

$$C_{CR}[\rho] \geq 4 \left( 1 - \frac{2|m|}{2L+1} \right) \langle r^2 \rangle \langle p^2 \rangle, \quad (4.4)$$

where  $L = l + \frac{d-3}{2}$  and  $l = 0, 1, 2, \dots$ . Then, taking into account the  $D$ -dimensional Heisenberg relation  $\langle r^2 \rangle \langle p^2 \rangle \geq (l + \frac{d}{2})^2 = (L + \frac{3}{2})^2$  for central potentials, we have [29] that

$$C_{CR}[\rho] \geq 4 \left( 1 - \frac{2|m|}{2L+1} \right) \left( L + \frac{3}{2} \right)^2. \quad (4.5)$$

Note that this lower bound equals to  $d^2$  for  $S$  states. Moreover, these inequalities behave as uncertainty relations although in the same space, indicating that the wigglier is the quantum-mechanical wavefunction of the system, the less concentrated around the centroid the associated probability density is, and vice versa.

Recently, a generalized version of the Crámer-Rao inequality involving a biparametric Fisher-information and Rényi entropy was proven by Lutwak et al. [119] for univariate distributions and by Bercher [120] and Lutwak et al [121] for multidimensional densities.

Furthermore, these Crámer-Rao inequalities have been generalized [119–121] as follows:

**Lemma 4.1.** [Crámer-Rao inequality for radially symmetric densities] [120]. *Let  $f(x) = f_r(|x|)$  be a radially symmetric probability density on the  $d$ -dimensional ball of radius  $R$ , possibly infinite, centered on the origin. Assume that the density is absolutely continuous and such that  $\lim_{r \rightarrow R} r^d f_r(r)^q = 0$ . Let also  $p \geq 1$  and  $p^*$  be its Hölder conjugate. Then, for  $q > d/(d + p^*)$  and provided that the involved information measures are finite, we*

have

$$F_{p,\lambda}[f]^{\frac{1}{p\Lambda}} \times \sigma_{p^*}[f] \geq K \equiv F_{p,\lambda}[g_{p,\lambda}]^{\frac{1}{p\Lambda}} \sigma_{p^*}[g_{p,\lambda}], \quad (4.6)$$

where  $\Lambda$  is given by  $\Lambda = 1 + (\lambda - 1)d$ , and  $g_{p,\lambda}$  denotes the  $(p, \lambda)$ -stretched deformed Gaussian distribution is defined by

$$g_{p,\lambda}(\vec{r}) \propto \begin{cases} \left(1 + (1 - \lambda)|\vec{r}|^{p^*}\right)_+^{\frac{1}{\lambda-1}}, & \text{for } \lambda \neq 1, \\ \exp\left(-|\vec{r}|^{p^*}\right), & \text{for } \lambda = 1, \end{cases} \quad (4.7)$$

where  $(\cdot)_+ = \max(\cdot, 0)$  (the case  $\lambda = 1$  is indeed obtained in the limit). The symbol  $\sigma_p[f]$  is the  $p$ -th typical deviation  $\sigma_p[f] = \langle |\vec{r}|^p \rangle^{\frac{1}{p}} = \int_{\mathbb{R}^d} |\vec{r}|^p f(\vec{r}) d\vec{r}$  (supposed a central density  $f$ ,  $\langle \vec{r} \rangle = 0$ ).

Later, in Sec 5.2 of this work we propose a novel biparametric version of the Crámer-Rao complexity measure for one-dimensional probability densities as

$$C_{p,\lambda}^{(CR)}[\rho] = \mathcal{K}_{p,\lambda}^{(CR)} \phi_{p,\lambda}[\rho] \times \sigma_p[\rho],$$

(where  $\phi_{p,\lambda}[\rho] = F_{p^*,\lambda}[\rho]^{\frac{1}{p^*\lambda}}$  as already defined) whose usefulness is illustrated by applying it to the blackbody radiation spectrum.

## 4.2 Measures of Fisher-Shannon type

The Fisher-Shannon measure of complexity, inspired by the Stam inequality [110], is defined [162, 241, 258] as

$$C_{FS}[\rho] := F[\rho] \times \frac{1}{2\pi e} e^{\frac{2}{a} S[\rho]}. \quad (4.8)$$

where  $F[\rho]$ , and  $e^{S[\rho]}$  denote the Fisher information and the the Shannon entropy power, respectively. Thus, it quantifies the combined balance of the gradient content of the density (i.e., the concentration of the quantum-mechanical probability cloud around the maxima of  $\rho(\vec{r})$ ) and the total spreading of the density all over its domain of definition. This quantity fulfills [7, 244] the inequality

$$C_{FS}[\rho] \geq d, \quad (4.9)$$

which saturates for the Gaussian density.

The Fisher-Shannon measure of complexity and the associated inequality have been generalized by using some generalizations of the standard Fisher information  $F[\rho]$  and/or the Shannon entropy  $S[\rho]$  (see e.g. [119–121, 225, 245, 251] such as the biparametric Fisher information  $F_{p,\lambda}[\rho]$  given by (1.19) and the Rényi entropy  $R_\lambda[\rho]$  given by (1.10), respectively.

Later in Sec. 5.1 of this work, a novel biparametric Fisher-Rényi complexity measure is introduced as

$$C_{p,\lambda}^{(FR)}[\rho] = \mathcal{K}_{p,\lambda}^{(FR)} \phi_{p,\lambda}[\rho] \times N_\lambda[\rho],$$

with  $\lambda > (p+1)^{-1}$  and where the symbols  $\mathcal{K}_{FR}(p, \lambda)$ ,  $\phi_{p,\lambda}[\rho]$  and  $N_\lambda[\rho]$  denote a normalization factor, the biparametric Fisher information [119] and the Rényi entropy power,  $N_\lambda[\rho] = \exp(R_\lambda[\rho])$ , respectively. This quantity includes the monoparametric one of Toranzo et al. [251] and the standard Fisher-Shannon complexity measure given by (4.8). Moreover, in Chapter 7, a family of tri-parametric complexity measures based on biparametric Fisher information and Rényi entropy are defined as

$$C_{p,\beta,\lambda}^{(FR)}[\rho] = \left( F_{p,\beta}[\rho]^{\frac{1}{p\beta}} N_\lambda[\rho] \right)^{2\beta},$$

which includes not only the above mentioned biparametric family but also some monoparametric Fisher-Rényi measures previously introduced in the literature [225, 237, 245, 259]. The exact sharp bound and the family of minimizing densities of these complexity measures are analytically obtained in Chapter 7.

### 4.3 Measures of LMC type

The LMC (Lopezruiz-Mancini-Calbet) complexity measure is defined [206, 213] as the product of the Shannon entropy power and the disequilibrium ( $\mathcal{D}[\rho] = e^{-R_2[\rho]}$ ), i.e.

$$C_{LMC}[\rho] := e^{S[\rho]} \mathcal{D}[\rho] = e^{S[\rho] - R_2[\rho]}. \quad (4.10)$$

Thus, it measures the combined balance of the average height of  $\rho(\vec{\mathbf{r}})$  and the total extent of the spread of the density over the whole hyperspace. This quantity satisfies the inequality [260]

$$C_{LMC}[\rho] \geq 1, \quad (4.11)$$

and possesses very interesting properties [61, 113, 205, 207, 218, 222, 236, 237, 239] such as e.g. the invariance under replication, translation and scaling transformations. Note that, contrary to the Crámer-Rao and Fisher-Shannon complexities which have a local-global character but in a different sense, the LMC complexity  $C_{LMC}[\rho]$  has a global-global character because it measures simultaneously two global spreading aspects of  $\rho(x)$ : the disequilibrium and the total extent of the density as given by the Shannon entropy power.

The LMC complexity has been applied to study the electronic structure of quantum systems [61, 113, 229, 240–242, 247, 261–263], confined systems [226, 264], chaotic regimes [228, 265], solids [266], the logistic map [214, 220], non-equilibrium systems [219, 224], hyperspherical harmonics [233, 234] and thermodynamics [235].

A natural biparametric extension of the LMC complexity, the so-called LMC-Rényi complexity measure, was introduced by Lopez-Ruiz et al. [208, 227] as

$$C_{\lambda,\beta}[\rho] = e^{R_\lambda[\rho] - R_\beta[\rho]}, \quad \lambda < \beta, \quad (4.12)$$

from which the plain LMC complexity measure (4.10) is recovered for  $\lambda = 1$  and  $\beta = 2$ . This quantity has been applied to the study of the electronic structure [60, 259], Fermi systems [246], ionization processes [243] and quantum phase transitions [250]. An extended, relative version of this quantity [231, 263] has been applied to the Dicke model and to some quantum-information objects (qubits, entangled states) [249].

Recently a modified version of this LMC-Rényi complexity measure defined by

$$\overline{C}_{\alpha,\beta}[\rho] := e^{\frac{1}{D}(R_\alpha[\rho] - R_\beta[\rho])}, \quad 0 < \alpha < \beta < \infty, \quad \alpha, \beta \neq 1. \quad (4.13)$$

has been shown to be most convenient in various contexts [34, 222, 225, 227, 267]. It keeps the same fundamental properties of the previous one, boils down to the plain LMC complexity measure  $C_{1,2}[\rho] = \mathcal{D}[\rho] \times e^{S[\rho]}$  when ( $\alpha \rightarrow 1, \beta = 2$ ) and fulfills the inequality

$$\overline{C}_{\alpha,\beta}[\rho] \geq 1 \quad \text{if} \quad \alpha < \beta \quad (4.14)$$

for  $D$ -dimensional probability densities. An approach to derive this universal lower bound is based on the well-known Jensen inequality [268] fulfilled by convex functions:

**Theorem 4.2.** *Let  $f(x), p(x)$  be two functions defined for  $a \leq x \leq b$  such that  $\alpha \leq f(x) \leq \beta$  and  $p(x) \geq 0$ , with  $p(x) \not\equiv 0$ . Let  $\phi(u)$  be a convex function defined on the interval  $\alpha \leq u \leq \beta$ ; then*

$$\phi \left( \frac{\int_a^b f(x)p(x) dx}{\int_a^b p(x) dx} \right) \leq \frac{\int_a^b \phi(f(x))p(x) dx}{\int_a^b p(x) dx}. \quad (4.15)$$

Note that by choosing  $p(x) = \rho(x)$ , a probability density, and (i) for  $\beta > \lambda > 1$ , ( $f(x) = [\rho(x)]^{\lambda-1}; \phi(u) = u^{\frac{\beta-1}{\lambda-1}}$ ), and (ii) for  $1 > \beta > \lambda$ , ( $f(x) = [\rho(x)]^{\beta-1}; \phi(u) = u^{\frac{\lambda-1}{\beta-1}}$ ), one directly obtains the sharp bound for the LMC-Rényi complexity measure  $C_{\lambda,\beta}[\rho] \geq 1$ , for any  $\lambda < \beta$ . Moreover, the family of minimizing densities turn out to be the uniform ones.

Later in Chapter 6 of this work, the LMC-Rényi complexity measure will be shown to have a monotonicity property through the use of the differential-escort transformation together with Jensen's inequality; special care will be taken for the extreme cases of minimal and maximal complexity.

Furthermore, for completeness, let us mention here that the three basic complexity measures (Crámer-Rao, Fisher-Shannon, LMC) can be bounded from above [175] so



that e.g. for real ( $d = 3$ ) quantum systems they satisfy the double inequalities

$$9 \leq C_{CR}[\rho] \leq 4\langle r^2 \rangle \langle p^2 \rangle, \quad (4.16)$$

$$3 \leq C_{FS}[\rho] \leq \frac{4}{3} \langle r^2 \rangle \langle p^2 \rangle, \quad (4.17)$$

and

$$1 \leq C_{LMC}[\rho] \leq \frac{2^{7/2}}{3^3 \sqrt{\pi}} e^{3/2} (\langle r^2 \rangle \langle p^2 \rangle)^{3/2}. \quad (4.18)$$

for the Cramér-Rao, Fisher-Shannon and LMC complexity measures, respectively. In fact, these upper bounds can be improved and generalized to  $d$ -dimensional quantum systems. Moreover, the lower bounds have been found to improve for real systems subject to a central quantum-mechanical potential [175].

Finally, let us point out that these inequalities get clearly improved either by taking into account some known data (as e.g. some power moments) or by referring to specific quantum systems (as e.g. the  $d$ -dimensional particle in a box [113], the  $d$ -dimensional rigid rotator [234] and the  $d$ -dimensional hydrogenic and oscillator-like systems [244]).

## Chapter 5

# Biparametric complexity measures: notion and application to the Planck distribution

### 5.1 Fisher-Rényi Complexity

In this section we define a novel class of generalized complexity measures for a general probability density  $\rho(x)$ , the biparametric Fisher-Rényi complexities  $C_{FR}^{(p,\lambda)}[\rho]$ . Basically these quantities are the product of two generalized entropic factors: the Rényi entropy power (that generalizes the Shannon entropy power) and the biparametric Fisher information. Thus, they jointly quantify the  $\lambda$ -dependent spreading aspects and the  $(p, \lambda)$ -dependent oscillatory facets of  $\rho(x)$ , so being much richer than the basic Fisher-Shannon complexity measure and its extensions of Fisher-Rényi type. Moreover we discuss the main properties of these complexity quantifiers (universal lower bound, scaling and translation invariance, monotonicity,...). Finally, we apply them to the  $d$ -dimensional blackbody radiation in standard ( $d = 3$ ) and non-standard ( $d \neq 3$ ) universes.

Specifically the following tasks have been done:

- We construct the family of biparametric Fisher-Rényi complexity measures  $C_{FR}^{(p,\lambda)}[\rho]$  for a general probability density  $\rho$ .
- We discuss the basic properties of these complexity quantifiers, including their behavior under replication transformation.
- We study both analytically and numerically the biparametric Fisher-Rényi complexity measure  $C_{FR}^{(p,\lambda)}[\rho_T^{(d)}]$  for the  $d$ -dimensional blackbody frequency distribution  $\rho_T^{(d)}(\nu)$  at temperature  $T$ . In particular we analyze their dependence on the involved parameters, including  $p, \lambda, d$  and  $T$ . It is found e.g. that the biparametric

Fisher-Rényi quantifier (i) does not depend on the temperature  $T$ , (ii) it has different behaviors according to the range of values of the pair  $(p, \lambda)$ .

These results have been published in the article [\[67\]](#) with coordinates:

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# The biparametric Fisher-Rényi complexity measure and its application to the multidimensional blackbody radiation

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In this work we first introduce a biparametric Fisher-Rényi complexity measure for general probability distributions and we discuss its properties. This notion, which is composed by two entropy-like components (the Rényi entropy and the biparametric Fisher information), generalizes the basic Fisher-Shannon measure and the previous complexity quantifiers of Fisher-Rényi type. Second, we illustrate the usefulness of this notion by carrying out an information-theoretical analysis of the spectral energy density of a  $d$ -dimensional blackbody at temperature  $T$ . It is shown that the biparametric Fisher-Rényi measure of this quantum system has a universal character in the sense that it does not depend on temperature nor on any physical constant (e.g., Planck constant, speed of light, Boltzmann constant), but only on the space dimensionality  $d$ . Moreover, it decreases when  $d$  is increasing, but exhibits a non trivial behavior for a fixed  $d$  and a varying parameter, which somehow brings up a non standard structure of the blackbody  $d$ -dimensional density distribution.

Keywords: Information theory, biparametric Fisher-Rényi complexity, Rényi entropy, biparametric Fisher information, black-body radiation, cosmic microwave background, generalized Planck distribution.

PACS:

## I. INTRODUCTION

General quantification of complexity attributed to many-body systems, the task which is closely connected with evolution from order to disorder, is among the most important scientific challenges in the theory of complex systems. The fundamental issue is to find one quantifier which is able to capture the intuitive idea that complexity lies between perfect order and perfect disorder. Most probably this idea cannot be formalized by a single complexity quantifier because of the so many facets of the term complexity. Based on Information Theory and Density Functional Theory, various computable and operationally meaningful density-dependent measures have been proposed: the entropy and complexity measures of the one-body probability density of the system. The former ones (mainly the Fisher information and the Shannon entropy, and their generalizations like Rényi and Tsallis entropies) capture a single macroscopic facet of the internal disorder of the system. The latter ones capture two or more macroscopic facets of the quantum probability density which characterize the system, being the most relevant ones up until now the complexity measures of Crámer-Rao, Fisher-Shannon and LMC (Lopez-ruiz-Mancini-Calvet), which are composed by two entropic factors. These three basic measures, which are dimensionless, have been shown to satisfy a number of interesting properties: bounded from below by unity [21,22], invariant under translation and scaling transformation [23,24], and monotone in a certain sense [13]. Recently, they have been generalized in various directions such as the measures of Fisher-Rényi [25,26,27,15,28] and LMC-Rényi [29,30,31,32] types.

The aim of this article is two-fold. First, we introduce a novel class of biparametric measures of complexities (namely, the generalized Fisher-Rényi measures) for continuous probability densities, which generalizes the basic Fisher-Shannon and some extensions of them of Fisher-Rényi [41–45]. Second, we apply these novel complexity quantifiers to the generalized Planck radiation law (1). Beyond the temperature, we will focus on the dependence of these quantifiers on the space dimensionality  $d$  and the complexity parameters.

The cosmic microwave, neutrino and gravitational backgrounds (cmb, cnb and cgb, respectively) give information about the universe at different times after the big bang. The cnb and cgb have been claimed to give information at one minute after the big bang and during the big bang, respectively, and to have been seen in recent experiments

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with controversial results, still under a careful examination [1–3] (see [4] for a brief summary). The cmb, originated at around 380 000 years after the big bang at a temperature of around 3000 Kelvin, is the only cosmic radiation background which is well established. It was first detected in 1964 by the antennae manipulation works of Penzias and Wilson [5], and later confirmed by satellite observations in a very detailed way [6–8]. It is known that the frequency distribution of the cmb which presently bathes our (three-dimensional) universe follows the Planck’s black body radiation law given by the (unnormalized) spectral density  $\rho_T^{(3)}(\nu) = \frac{8\pi h}{c^3} \nu^3 (e^{\frac{h\nu}{k_B T}} - 1)^{-1}$  at the temperature  $T_0 = 2.7255(6)$  Kelvin, where  $h$  and  $k_B$  denote the Planck and Boltzmann constants, respectively.

In the last few years there is an increasingly strong interest in the analysis of the quantum effects of the space dimensionality in the blackbody radiation [11–18] and, in general, for natural systems and phenomena of different types in various fields from high energy physics and condensed matter to quantum information and computation (see e.g. [19–28] and the monographs [29–32]). This is not surprising because of the fundamental role that the spatial dimensionality plays in the solutions of the associated wave equations [30, 31]. In the present work we adopt an information-theoretical approach to investigate the complexity effects of the spatial dimensionality in the spectral energy density per unit of frequency of a blackbody at temperature  $T$  which has been found [11–13] to be given in a  $d$ -dimensional space by the generalized Planck radiation law

$$\rho_T^{(d)}(\nu) = \frac{1}{\Gamma(d+1)\zeta(d+1)} \left(\frac{h}{k_B T}\right)^{d+1} \frac{\nu^d}{e^{\frac{h\nu}{k_B T}} - 1}, \quad (1)$$

(normalized to unity), where  $\Gamma(x)$  and  $\zeta(x)$  are the Euler gamma function and the Riemann zeta functions [9], respectively. This investigation will be done by means of a novel class of biparametric measures of complexity of Fisher-Rényi type which allows us to go further beyond the 2014-dated work [40] on the entropy-like measures of  $\rho_T^{(d)}(\nu)$  and the three basic two-component complexity measures of Crámer-Rao [33, 42], Fisher-Shannon [35, 36] and LMC (Lopez-ruiz-Mancini-Calvet)[37–39] types.

The structure of the work is the following. In section II the biparametric complexities and their entropy-like components (Rényi entropy, biparametric Fisher information) of a general continuous one-dimensional probability distribution are defined, and their meaning and properties relevant to this effort are briefly given and discussed. Then, in section III we determine and discuss the values of the previous entropy-like and complexity measures for the density  $\rho_T^{(d)}(\nu)$  which characterize the multidimensional blackbody distribution. Let us advance that the resulting blackbody biparametric complexities are mathematical constants (i.e. they are dimensionless), independent of the temperature  $T$  and of the physical constants (Planck’s constant, speed of light and Boltzmann’s constant), so that they only depend on the spatial dimensionality. Finally, some concluding remarks are given.

## II. THE BIPARAMETRIC FISHER-RÉNYI COMPLEXITY MEASURE OF A GENERAL DENSITY

In this Section we define and discuss the meaning of a class of biparametric complexity measures of Fisher-Rényi type for a one-dimensional continuous probability distribution  $\rho(x)$ ,  $x \in \Lambda \subseteq \mathbb{R}$ . Obviously it is assumed that the density is normalized to unity, so that  $\int_{\Lambda} \rho(x) dx = 1$ .

First, we define the biparametric Fisher-Rényi complexity measure of the density  $\rho(x)$  as

$$C_{FR}^{(p,\lambda)}[\rho] = \mathcal{K}_{FR}(p, \lambda) \phi_{p,\lambda}[\rho] \times N_{\lambda}[\rho], \quad p^{-1} + q^{-1} = 1, \quad \lambda > (p+1)^{-1}, \quad (2)$$

where the symbols  $\mathcal{K}_{FR}(p, \lambda)$ ,  $\phi_{p,\lambda}[\rho]$  and  $N_{\lambda}[\rho]$  denote a normalization factor, the biparametric Fisher information and the Rényi entropy power or Rényi entropic length,  $N_{\lambda}[\rho] = \exp(R_{\lambda}[\rho])$ , respectively. Moreover, the symbol  $R_{\lambda}[\rho]$  denotes the Rényi entropy of order  $\lambda$  is defined [48] as

$$R_{\lambda}[\rho] = \frac{1}{1-\lambda} \ln \left( \int_{\Delta} [\rho(x)]^{\lambda} dx \right); \quad \lambda > 0, \lambda \neq 1, \quad (3)$$

This quantity is known to quantify various  $\lambda$ -depending aspects of the probability spreading of the density  $\rho(x)$  all over its support  $\Lambda$ . In particular, when  $\lambda \rightarrow 1$  the Rényi entropy tends to the celebrated Shannon entropy  $S[\rho]$ , which measures the total spreading of  $\rho(x)$ . On the other hand, the biparametric Fisher information  $F_{p,\lambda}[\rho]$  given Lutwak

et al [47] by

$$\phi_{p,\lambda}[\rho] = \left( \int_{\Delta} |\rho(x)|^{\lambda-2} \rho'(x)^q \rho(x) dx \right)^{\frac{1}{q\lambda}}, \quad \frac{1}{p} + \frac{1}{q} = 1 \quad (4)$$

where  $p \in [1, \infty)$  and  $\lambda \in \mathbb{R}$ . Note that for the particular values  $(p, \lambda) = (2, 1)$  the square of this generalized measure reduces to the standard Fisher information, i.e.,  $\phi_{2,1}[\rho]^2 = F[\rho] = \int_{\Delta} \frac{|\rho'(x)|^2}{\rho(x)} dx$ . So, while  $F[\rho]$  quantifies the gradient content of  $\rho(x)$ , the generalized Fisher information  $\phi_{p,\lambda}[\rho]$  with  $p \neq 2$  and  $\lambda \neq 1$  measures the  $(p, \lambda)$ -depending aspects of the density fluctuations other than the gradient content.

And the normalization factor  $\mathcal{K}_{FR}(p, \lambda)$  in Eq. (2) is given by

$$\mathcal{K}_{FR}(p, \lambda) = (\phi_{p,\lambda}[G] N_{\lambda}[G])^{-1} = \left[ \frac{\lambda^{\frac{1}{q}}}{p^{\frac{1}{p}}} a_{p,\lambda} e_{\lambda} \left( \frac{-1}{p\lambda} \right)^{\frac{\lambda-1}{p} + 1} \right]^{\frac{1}{\lambda}} = a_{p,\lambda}^{\frac{1}{\lambda}} \left( \frac{(p\lambda + \lambda - 1)^{\frac{q\lambda - \lambda + 1}{q}}}{p\lambda^{\lambda}} \right)^{\frac{1}{\lambda - \lambda^2}}. \quad (5)$$

where  $G$  denotes the generalized Gaussian distribution  $G(x)$  [47] given by

$$G(x) = a_{p,\lambda} e_{\lambda}(|x|^p)^{-1} \quad (6)$$

where  $e_{\lambda}(x)$  denotes the modified  $q$ -exponential function [49]:

$$e_{\lambda}(x) = (1 + (1 - \lambda)x)^{\frac{1}{1-\lambda}}_+, \quad (7)$$

which for  $\lambda \rightarrow 1$  reduces to the standard exponential one,  $e_1(x) \equiv e^x$ . for  $p \in (0, \infty)$ ,  $\lambda > 1 - p$  and with the notation  $t_+ = \max\{t, 0\}$  for any real  $t$ ; the constant  $a_{p,\lambda}$  is given by

$$a_{p,\lambda} = \begin{cases} \frac{p(1-\lambda)^{1/p}}{2B(\frac{1}{p}, \frac{1}{1-\lambda} - \frac{1}{p})} & \text{if } \lambda < 1, \\ \frac{p}{2\Gamma(1/p)} & \text{if } \lambda = 1, \\ \frac{p(\lambda-1)^{1/p}}{2B(\frac{1}{p}, \frac{\lambda}{\lambda-1})} & \text{if } \lambda > 1. \end{cases} \quad (8)$$

Moreover, the symbol  $N_{\lambda}[G]$  denotes the Rényi entropic power of the generalized Gaussian distribution  $G(x)$  given by

$$N_{\lambda}[G] = \left[ a_{p,\lambda} e_{\lambda} \left( \frac{-1}{p\lambda} \right) \right]^{-1} \quad (9)$$

in which  $N_{\lambda}[G]$  and  $\phi_{p,\lambda}[G]$  represent the Rényi entropic power given in Eq. (9) and the biparametric Fisher information of the generalized Gaussian distribution [47] which, for  $1 \leq p \leq \infty$  and  $\lambda > \frac{1}{1+p}$ , the last quantity given by

$$\phi_{p,\lambda}[G] = \begin{cases} \frac{p^{\frac{1}{p\lambda}}}{\lambda^{\frac{1}{q\lambda}}} \left[ a_{p,\lambda} e_{\lambda} \left( \frac{-1}{p\lambda} \right)^{\frac{1}{q}} \right]^{\frac{\lambda-1}{\lambda}}, & p < \infty \\ 2^{(1-\lambda)/\lambda} \lambda^{\frac{-1}{\lambda}}, & p = \infty, \end{cases} \quad (10)$$

where  $a_{p,\lambda}$  is given in (8).

Note that, from (2), (3) and (4) we can state that the biparametric complexity measure  $C_{FR}^{(p,\lambda)}[\rho]$  quantifies the combined balance of the  $\lambda$ -dependent spreading facet of the probability distribution  $\rho(x)$  and the  $(p, \lambda)$ -dependent oscillatory facet of  $\rho(x)$ . It is then clear that this quantity is much richer than e.g. the Fisher-Shannon measure which quantifies a single spreading aspect of the distribution (namely, its total spreading given by the Shannon entropy power) together with a single oscillatory facet (which corresponds to the gradient content as given by the

standard Fisher information). Indeed the generalized complexity measure  $C_{FR}^{(p,\lambda)}[\rho]$  includes the basic Fisher-Shannon complexity measure [35, 36],  $C_{FS}[\rho] = \frac{1}{2\pi e} F[\rho] \exp(2S[\rho])$ , and the various one-dimensional complexity measures of Fisher-Rényi types recently published in the literature [41–45]. Most important is to point out that the novel complexity quantifier  $C_{FR}^{(p,\lambda)}[\rho]$  includes the one-parameter Fisher-Rényi complexity measure  $C_{FR}^{(\lambda)}$  [43], since

$$C_{FR}^{(\lambda)} = (C_{FR}^{(2,\lambda)})^{2\lambda}.$$

These two measures of complexity present a number of similarities and differences, which are worth to mention. First, following the lines of [43] it is straightforward to show that the biparametric measure, like the monoparametric one, has the following important properties: a universal unity lower bound ( $C_{FR}^{(p,\lambda)} \geq 1$ ), invariance under scaling and translation transformations and monotonicity. Moreover, the biparametric measure has the following behavior under replication transformation

$$C_{FR}^{(p,\lambda)}[\tilde{\rho}] = n^{\frac{1}{\lambda}} C_{FR}^{(p,\lambda)}[\rho]$$

where the density  $\tilde{\rho}$  representing  $n$  replications of  $\rho$  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  $\Lambda_m$  of each density  $\rho_m$  are disjoint. This property shows that this biparametric complexity quantifier, opposite to the monoparametric one, becomes replication invariant in the limit  $\lambda \rightarrow \infty$ ; this limiting property is an effect of the power  $\frac{1}{\lambda}$  which has the biparametric measure but not the monoparametric one. In this limit, the minimizer distribution of this complexity measure has the form of a Dirac-like delta. Moreover, this power effect provokes that the biparametric measure is well defined in the limit  $\lambda \rightarrow \infty$ , what does not happen in the monoparametric case. Another important difference between the bi- and uni-parametric complexity quantifiers is that the biparametric one has two degrees of freedom; this means that it does not only depend on  $\lambda$  but also on the parameter  $p$ . So, in particular when  $\lambda = 1$ , we can readily show that this quantifier is minimized for Freud-like probability distributions of the form  $e^{-|x|^p}$ , which has a great physical relevance in the theory of sub- and super-diffusive systems.

There exist many instances of the biparametric complexity measure  $C_{FR}^{(p,\lambda)}[\rho]$  which are relevant for different reasons. Let us just mention three of them. First, when  $\lambda > \frac{1}{1+p}$ ,  $\forall p > 0$ , we have that the resulting measure

$$C_{FR}^{[p]}[\rho] \equiv C_{FR}^{(p,1+\frac{1}{p})}[\rho]$$

is composed by two particularly relevant entropic factors: the generalized Fisher information

$$\phi_{p,1+\frac{1}{p}}[\rho] = \left( \int_{\Delta} |\rho'(x)|^q dx \right)^{\frac{1}{2q-1}},$$

which is a pure functional of the derivative of the density  $\rho$ , and the Rényi entropic power

$$N_{1+\frac{1}{p}}[\rho] = \left( \int_{\Delta} [\rho(x)]^{1+\frac{1}{p}} dx \right)^{-\frac{1}{p}} = \left\langle [\rho(x)]^{\frac{1}{p}} \right\rangle^{-p}$$

Moreover, this complexity measure is minimized by the distribution

$$e_{p,1+\frac{1}{p}}(x) = a_{p,1+\frac{1}{p}} \left( 1 - \frac{|x|^p}{p} \right)_+$$

Note furthermore that the support of this distribution is  $[-p^{\frac{1}{p}}, p^{\frac{1}{p}}]$ , which boils down to  $[-1, 1]$  for both values  $p = 1$  and  $p = \infty$ , and it becomes longest for  $p = e$ .

Second, when  $\lambda = 2$  the corresponding complexity measure  $C_{FR}^{(p,2)}[\rho]$  is proportional to the ratio  $\frac{\langle |\rho'(x)|^q \rangle^{\frac{1}{2q}}}{D[\rho]}$ , since the Fisher-information-factor is

$$\phi_{p,2}[\rho] = \left( \int_{\Delta} \rho(x) |\rho'(x)|^q dx \right)^{\frac{1}{2q}} = \langle |\rho'(x)|^q \rangle^{\frac{1}{2q}}$$

and the Rényi-entropic-power-factor is the inverse of the disequilibrium  $D(\rho)$  as

$$N_2[\rho] = \left( \int_{\Delta} [\rho(x)]^2 dx \right)^{-1} = D[\rho]^{-1}$$

Moreover, the resulting measure  $C_{FR}^{(p,2)}[\rho]$  is minimized by the distribution

$$e_{p,2}(x) = a_{p,2} (1 - |x|^p)_+.$$

Third, most remarkable, is that the measure in the limit  $p \rightarrow \infty$  is also well defined, corresponding to a step function  $\forall \lambda > 0$ . In the latter case the complexity measure is given by

$$C_{FR}^{(\infty,\lambda)} = \left( \frac{\lambda}{2} \right)^{\frac{1}{\lambda}} \phi_{\infty,\lambda}[\rho] N_{\lambda}[\rho].$$

where the generalized Fisher-like information  $\phi_{\infty,\lambda}[\rho]$  is given by

$$\phi_{\infty,\lambda}[\rho] = \left( \int_{\Delta} [\rho(x)]^{\lambda-1} |\rho(x)'| dx \right)^{\frac{1}{\lambda}}$$

(so that  $(\phi_{\infty,\lambda}[\rho])^{\lambda}$  corresponds to the total variation of  $\frac{\rho^{\lambda}}{\lambda}$  [47]) and  $N_{\lambda}[\rho]$  is the previously defined Rényi entropy power. The measure  $C_{FR}^{(\infty,\lambda)}$  has all the properties previously pointed out for the general biparametric Fisher-Rényi complexity. Moreover, it is minimized by the uniform distribution (as the basic LMC complexity). As well, within the set of all possible step-permutations of a generic distribution  $\rho$  composed of  $N$  step functions, the measure  $C_{FR}^{(\infty,\lambda)}$  gets minimized by all the monotonically increasing or decreasing distributions.

### III. THE BIPARAMETRIC FISHER-RÉNYI COMPLEXITY OF THE $d$ -DIMENSIONAL BLACKBODY

In this section, the biparametric Fisher-Rényi complexity measure  $C_{FR}^{(p,\lambda)}$  is investigated for the  $d$ -dimensional blackbody frequency distribution at temperature  $T$ ,  $\rho(\nu) \equiv \rho_T^{(d)}(\nu)$ , given by Eq. (1). It is given by

$$C_{FR}^{(p,\lambda)}[\rho_T^{(d)}] = \mathcal{K}_{FR}(p, \lambda) \phi_{p,\lambda}[\rho_T^{(d)}] \times N_{\lambda}[\rho_T^{(d)}], \quad \lambda p > \frac{d}{d-1} \quad (11)$$

where  $\mathcal{K}_{FR}(p, \lambda)$  is the normalization constant given by Eq. (5), and  $\phi_{p,\lambda}[\rho_T^{(d)}]$  and  $N_{\lambda}[\rho_T^{(d)}]$  are the generalized Fisher information and power Rényi entropy of the  $d$ -dimensional blackbody density, respectively, defined in the previous section whose values will be first expressed in the following.

The Rényi entropy power  $N_{\lambda}[\rho_T^{(d)}] = \exp\left(R_{\lambda}[\rho_T^{(d)}]\right)$ , where the Rényi entropy for the  $d$ -dimensional blackbody density defined in (3), has been shown [50] to be given by

$$R_{\lambda}[\rho_T^{(d)}] = \frac{1}{1-\lambda} \ln A_R(\lambda, d) + \ln\left(\frac{k_B T}{h}\right), \quad \lambda > 0, \lambda \neq 1 \quad (12)$$

where the constant  $A_R(\lambda, d)$  has the value

$$A_R(\lambda, d) = \frac{\Gamma(\lambda d + 1) \zeta_{\lambda}(\lambda d + 1, \lambda)}{\Gamma^{\lambda}(d + 1) \zeta^{\lambda}(d + 1)}. \quad (13)$$

with  $\lambda \in \mathbb{N} \setminus \{1\}$ , and the symbol  $\zeta_{\lambda}(s, a)$  denotes the modified Riemann zeta function (also known as Barnes zeta function) [51].

The biparametric Fisher information  $\phi_{p,\lambda}[\rho]$ , defined in (4), for the  $d$ -dimensional blackbody density at temperature  $T$  has been recently obtained [50] as

$$\phi_{p,\lambda}[\rho_T^{(d)}] = [A_F(p, \lambda, d)]^{\frac{1}{q\lambda}} \frac{h}{k_B T}, \quad q \in (1, \infty), \quad \lambda > 0, \quad \frac{1}{q} + \frac{1}{p} = 1 \quad (14)$$



where  $A_F(p, \lambda, d)$  denotes the proportionality constant,

$$A_F(p, \lambda, d) = \frac{I(q, \lambda, d)}{(\Gamma(d+1)\zeta(d+1))^{q\lambda-q+1}} \quad \text{with} \quad I(q, \lambda, d) = \int_{\mathbb{R}^+} \frac{x^{q(d\lambda-d-1)+d}}{(e^x-1)^{q\lambda+1}} |d(e^x-1) - xe^x|^q dx. \quad (15)$$

For  $d > \frac{\lambda p}{\lambda p - 1}$  (so that  $\phi_{p,\lambda}[\rho_T^{(d)}]$  is well-defined),  $q$  even and  $q\lambda \in \mathbb{N}$  the integral  $I(p, \lambda, d)$  in (15) is analytically solvable giving rise to the following value for the proportionality constant

$$A_F(p, \lambda, d) = \frac{\sum_{i=0}^q (-1)^{q-i} \binom{q}{i} d^i (\alpha d - i)! \zeta_{\alpha+q-i}(1 + \alpha d - i, \alpha)}{(\Gamma(d+1)\zeta(d+1))^\alpha}, \quad (16)$$

with  $\alpha \equiv q\lambda - q + 1$ . For the standard case ( $p = 2, \lambda = 1$ ) one obtains that

$$A_F(2, 1, d) = \frac{1}{2\zeta(d+1)} \left( \zeta(d) - \frac{d-3}{d-1} \zeta(d-1) \right), \quad d > 2 \quad (17)$$

The insertion of (12) and (14) into (11) allows us to obtain the following expression

$$C_{FR}^{(p,\lambda)}[\rho_T^{(d)}] = \mathcal{K}_{FR}(p, \lambda) A_F(p, \lambda, d)^{\frac{1}{q\lambda}} A_R(\lambda, d)^{\frac{1}{1-\lambda}} \quad (18)$$

for the biparametric Fisher-Rényi complexity measure of the  $d$ -dimensional black body at temperature  $T$ , where the constants  $A_R(p, \lambda, d)$  and  $A_F(\lambda, d)$  are given by Eqs. (13) and (15), respectively. Note that this two-parameter complexity quantifier does not depend on any physical constants (e.g., Boltzmann and Planck constants) but it does depend on the universe dimensionality only, thus having a universal character.

For a better understanding of how the biparametric Fisher-Rényi complexity measure  $C_{FR}^{(p,\lambda)}[\rho_T^{(d)}]$  is able to characterize the multidimensional blackbody distribution, we study its dependence on the spatial dimensionality  $d$  and the parameters  $p$  and  $\lambda$  in Figures 1 and 2. In Fig. 1 we represent the  $(p, \lambda)$ -chart of the Fisher-Rényi complexity for the three-dimensional blackbody distribution,  $C_{FR}^{(p,\lambda)}[\rho_T^{(3)}]$ , in terms of  $p$  and  $\lambda$ . This quantity has no physical units and it does not depend on the blackbody temperature, what highlights the universal character of the chart. Note that it captures a non-trivial entropic structure in the Planck distribution, which is quite smooth. Indeed, we observe that the Fisher-Rényi complexity (i) presents a relative minimal at around  $(p=?, \lambda=?)$ , (ii) increases for fixed  $\lambda$  when  $p$  is augmenting, and (iii) decreases to unity for fixed  $p$  when  $\lambda$  is increasing. This is possibly a consequence of a delicate balance between the distinct behavior of the distribution at the two extremes of the support, which contributes very differently to the two entropic factors of the Fisher-Rényi complexity. These phenomena can be also observed in the functions  $C_{FR}^{(2,\lambda)}[\rho_T^{(3)}]$  and  $C_{FR}^{(p,1)}[\rho_T^{(3)}]$  of Fig. 2, which correspond to the cuts at  $p = 2$  y  $\lambda = 1$  of the  $(p, \lambda)$ -chart, respectively.

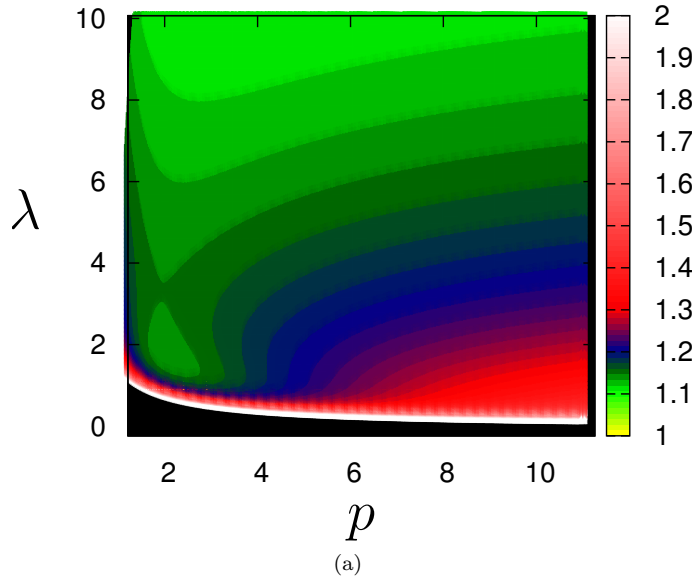


FIG. 1: Representation of the Fisher-Rényi complexity for the three-dimensional blackbody distribution,  $C_{FR}^{(p,\lambda)}[\rho_T^{(3)}]$ , in terms of  $p$  and  $\lambda$ .

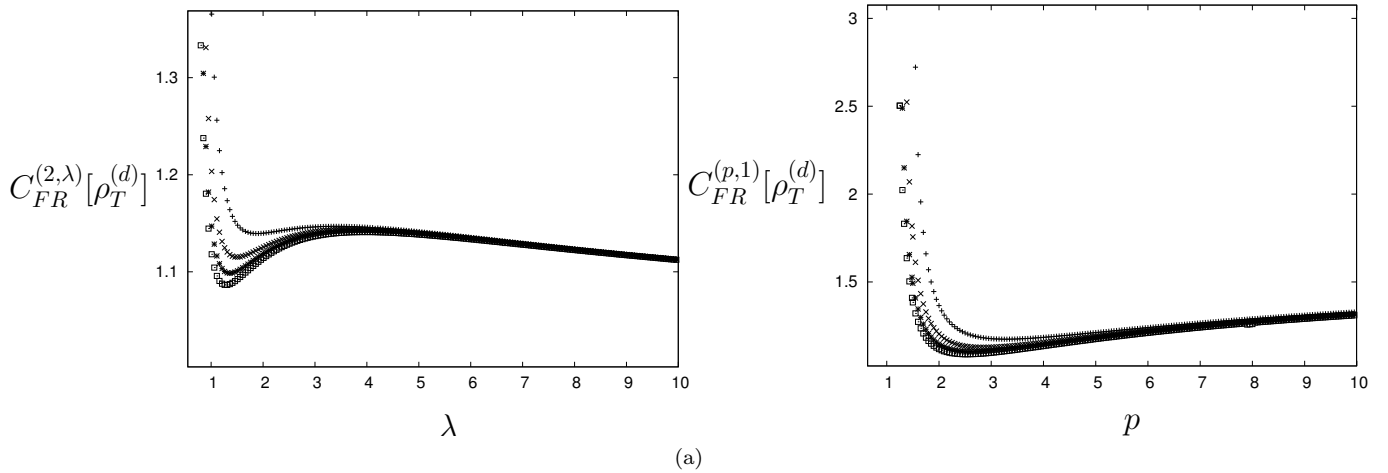


FIG. 2: Left: Dependence of the  $d$ -dimensional Fisher-Rényi complexity  $C_{FR}^{(2,\lambda)}[\rho_T^{(d)}]$  on  $\lambda$  when  $d = 3(+), 4(\times), 5(*), 6(\square)$ . Right: Dependence of the  $d$ -dimensional Fisher-Rényi complexity  $C_{FR}^{(p,1)}[\rho_T^{(d)}]$  on  $p$  when  $d = 3(+), 4(\times), 5(*), 6(\square)$ .

Besides we study in Fig. 2 the dimensionality dependence of the Fisher-Rényi complexity measures  $C_{FR}^{(2,\lambda)}[\rho_T^{(d)}]$  and  $C_{FR}^{(p,1)}[\rho_T^{(d)}]$  when  $d = 3(+), 4(\times), 5(*), 6(\square)$  in terms of the corresponding parameters  $\lambda$  and  $p$ , respectively. Note that the dimensionality behavior is qualitatively similar in each case. The complexity  $C_{FR}^{(2,\lambda)}[\rho_T^{(d)}]$  as a function of  $\lambda$  has for all dimensionalities a minimum and a maximum within the interval  $(0, 4)$  and then it monotonically decreases to unity. On the opposite, the complexity  $C_{FR}^{(p,1)}[\rho_T^{(d)}]$  as a function of  $p$  has only a minimum at  $p < 4$  for all dimensionalities and then it monotonically grows when  $p$  is increasing. In both cases the minimum location decreases when the dimensionality is augmenting. Quantitatively, we observe that for  $\lambda \geq 5$  in the left graph and for  $p \geq 4$  in the right graph the corresponding complexities do not practically depend on the dimensionality.

#### IV. CONCLUSIONS AND OPEN PROBLEMS

First we have shown in this paper that the Rényi entropy power,  $N_\lambda[\rho]$ , (that generalizes the Shannon entropy power) and the biparametric Fisher information,  $\phi_{p,\lambda}[\rho]$ , (which generalizes the standard Fisher information) allow us to construct a novel class of generalized complexity measures for a general probability density  $\rho(x)$ , the biparametric Fisher-Rényi complexities denoted by  $C_{FR}^{(p,\lambda)}[\rho]$ . They quantify the combined balance of the  $\lambda$ -dependent spreading aspects and the  $(p, \lambda)$ -dependent oscillatory facets of  $\rho(x)$ , so being much richer than the basic Fisher-Shannon measure and all its extensions of Fisher-Rényi type. Second, we have pointed out a number of properties of this quantifier, such as universal lower bound, scaling and translation invariance and monotonicity, among others. Third, we have applied these generalized measures of complexity to the  $d$ -dimensional blackbody radiation distribution at temperature  $T$ .

We have found that they do not depend on the temperature nor on the physical constants (Planck constant, speed of light and Boltzmann constant) but only on the spatial dimension, what gives them an universal character. We are aware that the full power of the novel complexity quantifier here proposed will be shown in multimodal probability distributions so abundant in natural phenomena such as e.g., the ones which are being observed in the modern observational missions of the cosmic microscopic background of the universe as well as the emergent frequency distributions of the cosmic neutrino and cosmic gravitational backgrounds (see e.g., [4]), the reason being that in such cases this quantifier may be used to detect and quantify the inherent anisotropies. Moreover, the use of this class of complexity quantifiers in fractal phenomena is being explored.

### Acknowledgments

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## 5.2 Crámer-Rao and Heisenberg-Rényi complexities

In this section we introduce two novel families of biparametric complexity measures of Crámer-Rao and Heisenberg-Rényi types for a general probability density, which extend the basic Crámer-Rao complexity measure and define a new family of complexity measures, respectively. Each family is basically composed by the product of a generalized dispersion measure of Heisenberg type (the so-called typical deviation of order  $p$ ) and a generalized entropic measure of Fisher (Crámer-Rao case) or Rényi (Heisenberg-Rényi case) type. Then, we discuss their main properties (invariance under scaling and translation transformations, lower-bounded by unity,...). Finally we apply these two novel complexity measures to the  $d$ -dimensional blackbody at temperature  $T$ . We have found that both types of quantifiers are universal constants in the sense that they are dimensionless and they do not depend on the temperature nor on any physical constant (such as e.g., Planck constant, speed of light or Boltzmann constant), so that they only depend on the spatial dimensionality of the universe. The results show the existence of a non trivial underlying mathematical structure, according to which these quantities become minimal for some values of their characteristic parameters.

Specifically the following tasks have been done:

- We construct the two families of biparametric complexity measures of Crámer-Rao and Heisenberg-Rényi types for a general probability density  $\rho$ .
- We discuss the basic properties of these complexity quantifiers, including their unity minimization by the generalized Gaussian densities.
- We determine these two complexity quantifiers to the generalized Planck frequency distribution of the blackbody radiation at temperature  $T$  in a  $d$ -dimensional universe. It is found that these two dimensionless quantities do not depend on  $T$  nor on any physical constants. So, they have an universal character in the sense that they only depend on the spatial dimensionality.
- To determine these blackbody complexity quantifiers we have calculated their dispersion (typical deviations) and entropy (Rényi entropies and the generalized Fisher information) constituents. They are found to have a temperature-dependent behavior similar to the celebrated Wien's displacement law of the dominant frequency  $\nu_{max}$  at which the spectrum reaches its maximum.

These results have been published in the article [68] with coordinates:

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# Biparametric complexities and the generalized Planck radiation law

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Complexity theory embodies some of the hardest, most fundamental and most challenging open problems in modern science. The very term *complexity* is very elusive, so that the main goal of this theory is to find meaningful quantifiers for it. In fact we need various measures to take into account the multiple facets of this term. Here some biparametric Crámer-Rao and Heisenberg-Rényi measures of complexity of continuous probability distributions are defined and discussed. Then, they are applied to the blackbody radiation at temperature  $T$  in a  $d$ -dimensional universe. It is found that these dimensionless quantities do not depend on  $T$  nor on any physical constants. So, they have an universal character in the sense that they only depend on the spatial dimensionality. To determine these complexity quantifiers we have calculated their dispersion (typical deviations) and entropy (Rényi entropies and the generalized Fisher information) constituents. They are found to have a temperature-dependent behavior similar to the celebrated Wien's displacement law of the dominant frequency  $\nu_{max}$  at which the spectrum reaches its maximum. Moreover, they allow us to gain insights into new aspects of the  $d$ -dimensional blackbody spectrum and about the quantification of quantum effects associated with space dimensionality.

Keywords: Biparametric measures of complexity of probability distributions, Information theory of the blackbody radiation in a multidimensional universe, cosmic microwave background, Planck distribution, Wien's law, disequilibrium, Shannon entropy, Fisher information, Crámer-Rao complexity, Fisher-Shannon complexity, LMC complexity, Heisenberg frequency, Shannon frequency, Fisher frequency.

## I. INTRODUCTION

The quantum many-body systems are not merely complicated in the way that machines are complicated but they are intrinsically complex in ways that are fundamentally different from any product of design. This intrinsic complexity makes them difficult to be fully described or comprehended. Moreover, in order to substantiate our intuition that complexity lies between perfect order and perfect disorder (i.e., maximal randomness), the ultimate goal of complexity theory is to find an operationally meaningful, yet nevertheless computable, quantifier of complexity. Many efforts have been done to understand it by using concepts extracted from information theory and density functional methods (see e.g., [1–4]). First, they used information entropies (Fisher information [5] and Shannon, Rényi and Tsallis entropies [6–8]) of the one-body densities which characterize the quantum states of the system. These quantities describe a single aspect of oscillatory (Fisher information) and spreading (Shannon, Rényi and Tsallis entropies) types of the quantum wavefunction. However, this is not enough to describe and quantify the multiple aspects of the complexity of natural systems from particle physics to cosmology [4, 9–12]. In fact there is no general axiomatic formalization for the term *complexity* (see a recent related effort [13]), but various quantifiers which take simultaneously into account two or more aspects of it. Most relevant up until now are the two-factor complexity measures of Crámer-Rao [14, 15], Fisher-Shannon [16, 17] and LMC (Lopez-ruiz-Mancini-Calvet)[18–20] types. They quantify the combined balance of two macroscopic aspects of the quantum probability density of the systems, and satisfy a number of interesting properties: dimensionless, bounded from below by unity [21, 22], invariant under translation and scaling transformation [23, 24]), and monotone in a certain sense [13]. Later on, some generalizations of these three basic quantities have been suggested which depend on one or two parameters, such as the measures of Fisher-Rényi [15, 25–28] and LMC-Rényi [29–32] types.

This article has two goals. First, we introduce two biparametric measures of complexities for continuous probability densities, which are qualitatively different from all the previously known ones, generalizing some of them (Crámer-Rao, LMC); namely, the generalized Crámer-Rao (or Fisher-Heisenberg) and the Heisenberg-Rényi measures. Then, we discuss their main properties. Second, we apply these two complexity measures to the generalized Planck radiation law, which gives the spectral frequency density of a blackbody at temperature  $T$  in a  $d$ -dimensional universe. This quantum object has played a fundamental role since the pionnering works of Planck at the birth of quantum mechanics up until now from both theoretical [33–43] and experimental [44–48] standpoints. Keep in mind e.g. that the cosmic microwave background radiation which bathes our universe today is known to be the most perfect blackbody radiation ever observed in nature, with a temperature of about 2.7255(6) Kelvin [47–50]. Beyond the temperature, we will focussed on the dependence of the complexity quantities on the space dimensionality

$d$ ; mainly, because this variable is crucial in the analysis of the structure and dynamics of natural systems and phenomena from condensed matter to high energy physics, cosmology and quantum information (see e.g. [51–58] and the monographs [59–62]). The  $d$ -dependence of the entropy-like and complexity-like quantities of the  $d$ -dimensional hydrogenic and harmonic systems has been recently reviewed [51] up until 2012, and more recently the three basic complexity measures (Crámer-Rao, Fisher-Shannon and LMC) of the  $d$ -dimensional blackbody have been shown to have an universal character in the sense that they depend neither on temperature nor on the Planck and Boltzmann constants, but only on the space dimensionality  $d$ . In this work, we will prove that a similar statement can be argued for the two biparametric measures of complexity mentioned above.

The structure of the article is the following. In section II some spreading quantities (typical deviations, Rényi entropy, biparametric Fisher information) of a general continuous one-dimensional probability distribution are considered, and their meanings and properties relevant to this work are briefly given and discussed. In addition, two biparametric complexity measures of Crámer-Rao and Heisenberg-Rényi character are defined in terms of the previous spreading quantities. In Section III the central moments, Rényi entropy and generalized Fisher information are studied analytically and numerically for the  $d$ -dimensional blackbody spectrum in terms of its temperature and the space dimensionality. This research allows to conclude that these measures could be used as quantifiers of the spatial anisotropy whose details are being investigated at present in a more precise way with the most modern astronomical tools. In particular, the generalized Fisher information (due to its strong sensitivity to the spectrum fluctuations) could contribute to the elucidation of the origin of the cosmic microwave background anisotropies.

Then, in section IV the generalized measures of complexity of the blackbody spectrum are investigated, finding that the biparametric complexities (Crámer-Rao and Heisenberg-Rényi) of the  $d$ -dimensional blackbody are dimensionless and, moreover, they do not depend on the temperature  $T$  of the system nor on any physical constant (e.g., Planck's constant, speed of light, Boltzmann's constant). Thus, they are universal quantities since they only depend on the spatial dimensionality.

Finally, in section V some concluding remarks are given, and various open problems are pointed out relative to the new complexity measures as well as the frequency distribution of a tri- and  $d$ -dimensional blackbody in order to shed some more light on the knowledge of the radiation that bathes our universe.

## II. BASIC AND EXTENDED MEASURES OF COMPLEXITY

In this Section first we briefly give the three basic complexity measures of a probability distribution; namely, the Crámer-Rao, Fisher-Shannon and LMC complexities. Then, we define two novel families of complexity measures (the biparametric Crámer-Rao and Heisenberg-Rényi complexities) which generalize the previous ones.

### A. Basic complexities

Let us consider a general one-dimensional random variable  $X$  characterized by the continuous probability distribution  $\rho(x)$ ,  $x \in \Lambda \subseteq \mathbb{R}$ . Obviously it is assumed that the density is normalized to unity, so that  $\int_{\Lambda} \rho(x) dx = 1$ . The basic measures of complexity of Crámer-Rao, Fisher-Shannon and LMC types are defined by means of the expressions

$$C_{CR}[\rho] = F[\rho] V[\rho], \quad (1)$$

$$C_{FS}[\rho] = \frac{1}{2\pi e} F[\rho] \exp(2S[\rho]), \quad (2)$$

$$C_{LMC}[\rho] = D[\rho] \exp(S[\rho]), \quad (3)$$

respectively. The symbols  $F[\rho]$ ,  $V[\rho]$ ,  $S[\rho]$ , and  $D[\rho]$  denote the standard Fisher information [3, 5]

$$F[\rho] = \int_{\Delta} \frac{|\rho'(x)|^2}{\rho(x)} dx, \quad (4)$$

the variance (see e.g. [63])

$$V[\rho] = \langle x^2 \rangle - \langle x \rangle^2; \quad \langle f(x) \rangle = \int_{\Delta} f(x) \rho(x) dx, \quad (5)$$

the Shannon entropy [6]

$$S[\rho] = - \int_{\Delta} \rho(x) \ln[\rho(x)] dx, \quad (6)$$



and the disequilibrium [64]

$$D[\rho] = \int_{\Delta} [\rho(x)]^2 dx, \quad (7)$$

of the probability density  $\rho(x)$ , respectively. The Fisher information quantifies the gradient content or pointwise concentration of the probability over its support interval  $\Lambda$ . The variance, the Shannon entropy and the disequilibrium measure the following spreading properties of  $\rho(x)$ : the concentration of the density around the centroid  $\langle x \rangle$ , the total extent to which the density is in fact concentrated, and the separation of the density with respect to equiprobability, respectively. Note that the Fisher information has a property of locality because it is very sensitive to the fluctuations of the density, contrary to the three spreading quantities which have a global character because they are power functionals of the density. The property of locality is very important in the quantum-mechanical description of physical systems, because their associated wavefunctions are inherently oscillatory for all quantum states except at the ground case.

Therefore, the Crámer-Rao, Fisher-Shannon and LMC complexities of  $\rho(x)$  are statistical measures of complexity which quantify the combined balance of two aspects of the density described by their two associated spreading components of dispersion and entropic character. Both the Crámer-Rao and Fisher-Shannon complexities have a local-global character but in a different sense: The Crámer-Rao complexity  $C_{CR}[\rho]$  quantifies the gradient content of  $\rho(x)$  and the probability concentration around its centroid, and the Fisher-Shannon complexity  $C_{FS}[\rho]$  measures the gradient density jointly with the total extent of the density in the support interval as given by the squared Shannon entropy power. The LMC complexity  $C_{LMC}[\rho]$  has a global-global character because it measures simultaneously two global spreading aspects of  $\rho(x)$ : the disequilibrium and the total extent of the density as given by the Shannon entropy power. These three dimensionless complexity measures are known to be bounded from below by unity [21, 22], and invariant under translation and scaling transformation [23, 24]. The question whether these quantities are minimum for the two extreme (or *least complex*) distributions corresponding to perfect order and maximum disorder (associated to an extremely localized Dirac delta distribution and a highly flat distribution in the one dimensional case, respectively) is a long standing and controverted issue [32, 65] which has been partially solved. Indeed, these three statistical measures have been recently shown to be monotone in a well-defined sense [13].

## B. Extended complexities

Now, inspired by Lutwak et al' efforts [66], we introduce two generalized statistical measures of complexity of local-global character (the biparametric Crámer-Rao or Fisher-Heisenberg and Heisenberg-Rényi complexities) which extend the basic complexity measures mentioned above. For this purpose we take into account the  $p$ th-typical deviation (or  $p$ th absolute deviation with respect to the middle value)  $\sigma_p[\rho]$  of the probability density  $\rho(x)$  defined as

$$\sigma_p[\rho] = \begin{cases} e^{\int_{\Delta} \rho(x) \ln |x - \langle x \rangle| dx}, & \text{if } p = 0 \\ \left( \int_{\Delta} |x - \langle x \rangle|^p \rho(x) dx \right)^{\frac{1}{p}}, & \text{if } 0 < p < \infty \\ \text{ess sup}\{|x - \langle x \rangle| : \rho(x) > 0\}, & \text{if } p = \infty \end{cases} \quad (8)$$

and the Rényi entropic power defined as

$$N_{\lambda}[\rho] = e^{R_{\lambda}[\rho]}, \quad (9)$$

where  $R_{\lambda}[\rho]$  denotes the standard or monoparametric Rényi entropy of order  $\lambda$  [7] given by

$$R_{\lambda}[\rho] = \frac{1}{1 - \lambda} \ln \left( \int_{\Delta} [\rho(x)]^{\lambda} dx \right); \quad \lambda > 0, \lambda \neq 1. \quad (10)$$

Note that the the  $p$ -typical deviations quantify different facets (governed by the parameter  $p$ ) of the concentration of the probability density around the centroid, and the  $\lambda$ -Rényi entropic powers measure various aspects (governed by

$\lambda$ ) of the global spreading of the probability density along its support interval. In particular we have that

$$N_\lambda[\rho] = \begin{cases} \text{Length of the support,} & \text{if } \lambda = 0 \\ e^{-\langle \ln \rho \rangle}, & \text{if } \lambda = 1 \\ \langle \rho \rangle^{-1} & \text{if } \lambda = 2 \\ \rho_{max}^{-1}, & \text{if } \lambda \rightarrow \infty. \end{cases}$$

It is also worth to realize the well-known fact that, when  $\lambda$  tends to unity, the Rényi entropy  $R_\lambda[\rho]$  tends to the Shannon entropy  $S[\rho]$ .

Besides, to define the novel complexity quantifiers we need to consider the (scarcely known) biparametric  $(p, \lambda)$ -Fisher information [66] defined as

$$\phi_{p,\lambda}[\rho] = \begin{cases} \text{ess sup}\{|\rho(x)^{\lambda-2}\rho'(x)|^{\frac{1}{\lambda}} : x \in \Delta\}, & \text{if } p = 1 \\ (\int_\Delta |\rho(x)^{\lambda-2}\rho'(x)|^q \rho(x) dx)^{\frac{1}{q\lambda}}, & 1 < p < \infty, = 1 \\ \left(\text{Total variation of } \frac{\rho(x)^\lambda}{\lambda}\right)^{\frac{1}{\lambda}}, & p \rightarrow \infty \end{cases} \quad (11)$$

with  $\frac{1}{p} + \frac{1}{q} = 1$ ,  $p \in (1, \infty)$ , and  $\lambda \in \mathbb{R}$ . Note that for the particular values  $(p, \lambda) = (2, 1)$ , this generalized measure reduces to the standard Fisher information  $F[\rho]$  in the sense that  $\phi_{2,1}[\rho]^2 = F[\rho]$ . It is then clear that the  $(p, \lambda)$ -Fisher informations quantify various fluctuation-like facets (governed by the parameters  $p$  and  $\lambda$ ) of the probability density  $\rho(x)$ , including the gradient content (when  $p = 2$  and  $\lambda = 1$ ).

The biparametric  $(p, \lambda)$ -Crámer-Rao (also called by biparametric Fisher-Heisenberg) complexity is defined as

$$C_{CR}^{(p,\lambda)}[\rho] = \mathcal{K}_{CR}(p, \lambda) \phi_{p,\lambda}[\rho] \sigma_p[\rho], \quad (12)$$

where  $1 \leq p \leq \infty$  and  $\lambda > \frac{1}{1+p}$ , and the symbols  $\sigma_p[\rho]$  and  $\phi_{p,\lambda}[\rho]$  denote the typical deviation of order  $p$  and the Fisher information of order  $(p, \lambda)$ , respectively, previously defined. Moreover, the constant  $\mathcal{K}_{CR}(p, \lambda)$  is given by

$$\mathcal{K}_{CR}(p, \lambda) = \frac{1}{\phi_{p,\lambda}[G] \sigma_p[G]} \quad (13)$$

where the  $\phi_{p,\lambda}[G]$  and  $\sigma_p[G]$  denote the values of the  $(p, \lambda)$ th-Fisher information and the  $p$ th-order typical deviation of the generalized Gaussian density  $G(x) \equiv G_{p,\lambda}(x)$  defined as [66]

$$G(x) = a_{p,\lambda} e_\lambda(|x|^p)^{-1} \quad (14)$$

for  $p \in [0, \infty]$  and  $\lambda > 1 - p$ . The symbol  $e_\lambda(x)$  denotes the modified  $\lambda$ -exponential function:

$$e_\lambda(x) = (1 + (1 - \lambda)x)_+^{\frac{1}{1-\lambda}}, \quad (15)$$

where the notation  $t_+ = \max\{t, 0\}$  for any real  $t$  has been used. Note that for  $\lambda \rightarrow 1$  it reduces to the standard exponential one,  $e_1(x) \equiv e^x$ . Moreover, the normalization constant  $a_{p,\lambda}$  has the value

$$a_{p,\lambda} = \begin{cases} \frac{p(1-\lambda)^{1/p}}{2B\left(\frac{1}{p}, \frac{1}{1-\lambda} - \frac{1}{p}\right)} & \text{if } \lambda < 1, \\ \frac{p}{2\Gamma(1/p)} & \text{if } \lambda = 1, \\ \frac{p(\lambda-1)^{1/p}}{2B\left(\frac{1}{p}, \frac{\lambda}{\lambda-1}\right)} & \text{if } \lambda > 1, \end{cases}$$

where the symbol  $B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$  denotes the known Beta function [69] and an errata has been corrected for the  $(\lambda > 1)$ -case: it is not  $B\left(\frac{1}{p}, \frac{1}{1-\lambda}\right)$  as in [66], but  $B\left(\frac{1}{p}, \frac{\lambda}{\lambda-1}\right)$ . Note that the properties of the generalized Gaussian density are carefully detailed in Sect. II-E of [66]; other, more recent, expressions of this generalized density function and their corresponding properties have been shown (see e.g., [67, 68]).

On the other hand, the constant values  $\phi_{p,\lambda}[G]$  and  $\sigma_p[G]$  are given by

$$\phi_{p,\lambda}[G] = \begin{cases} p^{\frac{1}{\lambda}} a_{p,\lambda}^{\frac{\lambda-1}{\lambda}} (p\lambda + \lambda - 1)^{-\frac{(1-\frac{1}{p})}{\lambda}}, & p < \infty \\ 2^{(1-\lambda)/\lambda} \lambda^{\frac{-1}{\lambda}}, & p \rightarrow \infty \end{cases} \quad (16)$$

and

$$\sigma_p[G] = \begin{cases} (p\lambda + \lambda - 1)^{-1/p}, & p \in (0, \infty), \lambda > \frac{1}{1+p} \\ e^{\frac{\lambda}{1-\lambda}}, & p = 0, \lambda > 1 \\ 1 & p \rightarrow \infty, \end{cases} \quad (17)$$

respectively. Note that the case  $(p = 2, \lambda = 1)$  corresponds to the basic Crámer-Rao measure  $C_{CR}[\rho]$  given by (1). From its definition (12), we observe that the biparametric Crámer-Rao or Fisher-Heisenberg complexity quantifies the combined balance of a fluctuation aspect of the density (as given by the generalized Fisher information which depends on the parameters  $p$  and  $\lambda$ ; this aspect is the gradient content in the particular case  $p = 2, \lambda = 1$ ) and a dispersion facet of the probability concentration with respect to the centroid (as given by the central moment of order  $p$ ; this aspect is the variance of the density in the particular case  $p = 2$ ).

The biparametric  $(p, \lambda)$ -Heisenberg-Rényi complexity is defined as

$$C_{HR}^{(p,\lambda)}[\rho] = \mathcal{K}_{HR}(p, \lambda) \frac{\sigma_p[\rho]}{N_\lambda[\rho]} \quad (18)$$

where  $\lambda \neq 1$ ,  $0 \leq p \leq \infty$  and  $\lambda > \frac{1}{1+p}$ , and the symbols  $\sigma_p[\rho]$  and  $N_\lambda[\rho]$  denote the  $p$ th-typical deviation (8) and the Rényi entropic power, respectively, previously defined. Moreover, the constant  $\mathcal{K}_{HR}(p, \lambda)$  has the value

$$\mathcal{K}_{HR}(p, \lambda) = \frac{N_\lambda[G]}{\sigma_p[G]}, \quad (19)$$

where the symbol  $N_\lambda[G]$  denotes the Rényi entropic power of the generalized Gaussian density [66] is given by

$$N_\lambda[G] = \left( a_{p,\lambda} e_\lambda \left( \frac{-1}{p\lambda} \right) \right)^{-1} \quad (20)$$

and the symbols  $a_{p,\lambda}$  and  $\sigma_p[G]$  have been previously given.

We realize from (18) that the biparametric  $(p, \lambda)$ th-Heisenberg-Rényi complexity quantifies the combined balance of a dispersion aspect of the probability concentration with respect to the centroid (as given by  $p$ th-typical deviation  $\sigma_p[G]$ , which is the standard deviation of the density in the particular case  $p = 2$ ) and the global spreading of the density (as given by the Rényi entropic power of order  $\lambda$ , which boils down to the Shannon entropic power in the particular case  $\lambda \rightarrow 1$ ).

These two biparametric statistical complexities turns out to be invariant under scaling and translation transformations and lower-bounded by unity, as implicitly shown in [66]; moreover, the equality to unity occurs at the generalized Gaussian densities given by (14).

To get a further insight into the type of densities  $G_{p,\lambda}(x)$  which minimize the two previous families of extended complexities, we have indicated in Fig. 1 the kind of relevant distributions which correspond to a large set of values for the parameters  $(p, \lambda)$ . Let us only mention the standard Gaussian distribution, the exponential, the  $q$ -exponential, the linear, the Cauchy, the logarithmic and the ladder distributions which are particular cases of generalized Gaussian distributions with  $(p, \lambda) = (2, 1), (1, 1), (1, q), (1, 2), (0, 2), (2, 0)$  and  $(\infty, \lambda)$ , respectively. More important is to note that the behavior of the tail of the distribution is closely related to  $\lambda$ , so that the minimizer distribution of the complexities correspond to a compact-support distribution, a light-tailed distribution (i.e., one with infinite support and all its moments finite) and a heavy-tailed distribution for the cases  $\lambda > 1$ ,  $\lambda = 1$  and  $\lambda < 1$ , respectively. Thus, since Gaussianity occurs for minimal complexities, the two novel measures of complexity provide a relevant information about the relative behavior of different regions of the distribution. This is illustrated elsewhere for some specific quantum systems of Coulombic and harmonic character. Here we show in the next section the usefulness of these measures of complexity by evaluating them for the generalized Planck distribution which governs the distribution of radiation frequencies of a blackbody at temperature  $T$  in a universe of arbitrary dimensionality.

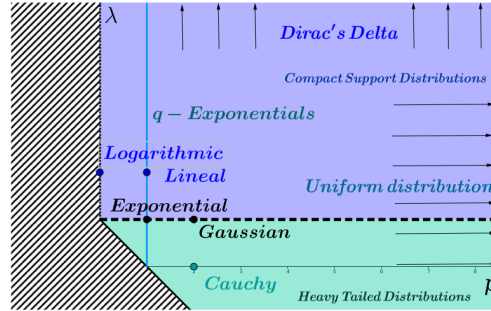


FIG. 1: The Gaussian  $(p, \lambda)$  plane.

### III. APPLICATION TO THE GENERALIZED PLANCK RADIATION LAW

In this section we extend the information-theoretic study of a  $d$ -dimensional ( $d > 1$ ) blackbody at temperature  $T$ , initiated last year [42], by calculating the measures of dispersion (typical deviations of order  $p$ ) beyond the standard one (i.e., that with  $p = 2$ ), the spreading quantities given by the Rényi entropic powers (which include the Shannon entropic power as a particular case), the generalized Fisher informations (which includes the standard Fisher information as a particular case) and the two biparametric complexity measures introduced in the previous section (which generalize the three basic measures of complexity mentioned above) of its spectral energy density  $\rho_T^{(d)}(\nu)$  (i.e., the energy per frequency and volume units contained in the frequency interval  $(\nu, \nu + d\nu)$  inside a  $d$ -dimensional enclosure maintained at temperature  $T$ ), which is given by the (normalized-to-unity) generalized Planck radiation law [33, 34] (see also [42])

$$\rho_T^{(d)}(\nu) = \frac{1}{\Gamma(d+1)\zeta(d+1)} \left( \frac{h}{k_B T} \right)^{d+1} \frac{\nu^d}{e^{\frac{h\nu}{k_B T}} - 1}, \quad (21)$$

where  $h$  and  $k_B$  are the Planck and Boltzmann constants, respectively, and  $\Gamma(x)$  and  $\zeta(x)$  denote the Euler's gamma function and the Riemann's zeta function[69], respectively.

#### A. Typical deviations

Let us first determine the typical deviations  $\sigma_p[\rho_T^{(d)}]$  of the  $d$ -dimensional blackbody density  $\rho_T^{(d)}(\nu)$  defined as

$$\sigma_p[\rho_T^{(d)}]^p = A \int_0^\infty |\nu - \langle \nu \rangle|^p \frac{\nu^d}{e^{a\nu} - 1} d\nu, \quad (22)$$

with the notation

$$A = \frac{1}{\Gamma(d+1)\zeta(d+1)} a^{d+1}, \quad a = \frac{h}{k_B T}.$$

Since the centroid of the density has the value

$$\langle \nu \rangle = (d+1) \frac{\zeta(d+2)}{\zeta(d+1)} \frac{1}{a} \equiv \frac{b}{a},$$

we obtain that the typical deviation of even order  $p$  of the blackbody depends on temperature  $T$  as

$$\sigma_p[\rho_T^{(d)}] = (A_H(p, d))^{\frac{1}{p}} \frac{k_B T}{h}, \quad (23)$$

where the proportionality constant is given by

$$\begin{aligned} A_H(p, d) &= \sum_{n=0}^p (-1)^{p-n} \binom{p}{n} \left( (d+1) \frac{\zeta(d+2)}{\zeta(d+1)} \right)^{p-n} \frac{\Gamma(d+n+1)}{\Gamma(d+1)} \frac{\zeta(d+n+1)}{\zeta(d+1)} \\ &\equiv \sum_{n=0}^p \gamma_n(p, d) \zeta(d+n+1), \end{aligned} \quad (24)$$

which only depends on the space dimensionality  $d$ . We observe that all  $p$ -typical deviations follow a Wien-like law, in the sense that they are directly proportional to the temperature of the system. In Fig. 2 we plot the  $p$ -dependence of  $\sigma_p[\rho_T^{(d)}] \frac{h}{k_B T}$  for various dimensionalities of the universe, finding a linearly increasing behavior when  $p$  is augmenting. Moreover, we note that the increasing of the space dimensionality provokes a larger dispersion of the radiation frequencies with respect to the middle value.

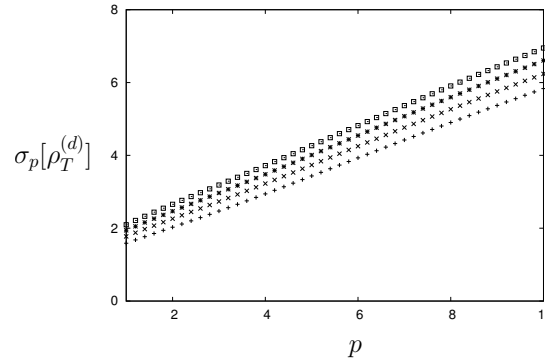


FIG. 2: Dependence of the  $p$ th-typical deviation,  $\sigma_p[\rho_T^{(d)}]$  in  $\frac{h}{k_B T}$ -units, on the parameter  $p$  for the universe dimensionalities  $d = 3(+), 4(\times), 5(*), 6(\square)$ .

## B. Rényi entropies

Let us now calculate the Rényi entropic power  $N_\lambda[\rho_T^{(d)}] = e^{R_\lambda[\rho_T^{(d)}]}$ , given by (9), of the multidimensional blackbody density (21) at temperature  $T$ , where the  $\lambda$ -Rényi entropy is given by

$$R_\lambda[\rho_T^{(d)}] = \frac{1}{1-\lambda} \ln \left( \int_{\Delta} [\rho_T^{(d)}]^\lambda d\nu \right); \quad \lambda > 0, \lambda \neq 1. \quad (25)$$

Taking into account Eqs. (9) and (10) and the corollary of the Lemma proved in Appendix V, we obtain that

$$N_\lambda[\rho_T^{(d)}] = A_R(\lambda, d)^{\frac{1}{1-\lambda}} \frac{k_B T}{h}, \quad (26)$$

with  $\lambda > 0, \lambda \neq 1$ , and the proportionality constant

$$A_R(\lambda, d) = \frac{\Gamma(\lambda d + 1) \zeta_\lambda(\lambda d + 1, \lambda)}{[\Gamma(d+1) \zeta(d+1)]^\lambda}, \quad (27)$$

where the symbol  $\zeta_n(s, a) \equiv \zeta_n(s, a|1, \dots, 1)$  denotes the modified Riemann zeta function or Barnes zeta function [70, 71], defined for  $n \in \mathbb{N}$ , which for  $a \neq 0, -1, -2, \dots$  is known to have the integral representation, when  $\text{Re}(s) > n$ :

$$\begin{aligned}\zeta_n(s, a) &= \frac{1}{\Gamma(s)} \int_0^\infty \frac{x^{s-1} e^{(n-a)x}}{(e^x - 1)^n} dx \\ &= \sum_{j=0}^{n-1} q_{n,j}(a) \zeta(s - j, a),\end{aligned}$$

with the coefficients [71]

$$q_{n,j}(a) = \frac{1}{(n-1)!} \sum_{l=j}^{n-1} (-1)^{n+l-1} \binom{l}{j} S_{n-1}^{(l)} (1-a)^{l-j}, \quad (28)$$

where  $S_n^{(l)}$  are the well-known Stirling's numbers of the first kind. The symbol  $\zeta(s, a)$  denotes the known Hurwitz's zeta function [69] so that for  $a = 1$  it boils down to the standard Riemann's zeta function  $\zeta(s)$ . Furthermore, it is shown in Appendix V that the Barnes' zeta function can be expressed as

$$\zeta_n(s, a) = \sum_{j=0}^{n-1} q_{n,j}(a) \zeta(s - j, a - 1) = \sum_{j=0}^{n-1} q_{n,j}(a) \zeta(s - j),$$

as far as  $a \in \mathbb{N}$ . In general the Barnes function is also known as the multiple (or  $n$ th-order) Hurwitz zeta function given by

$$\zeta_n(s, a|\omega_1, \dots, \omega_n) = \sum_{k_1, \dots, k_n=0}^{\infty} \frac{1}{(\Omega + a)^s},$$

with  $\text{Re}(s) > n$ ;  $n \in \mathbb{N}$  and where  $\Omega = k_1\omega_1 + \dots + k_n\omega_n$ . This function was first introduced by Barnes in 1899 [70] (who also gives the general conditions to be fulfilled by the parameters  $a$  and  $\omega_i$ ,  $i \in \mathbb{N}$ ; see also [71]) in his study of the multiple (or  $n$ th-order) gamma functions, whose physico-mathematical relevance was discovered in 1980 on the study about the determinants of the Laplacians on the  $n$ -dimensional unit sphere.

Note from (26) that the  $\lambda$ th-Rényi entropic power, which has units of frequency, follows a Wien's like displacement law in the sense that it linearly depends on the blackbody temperature. In Fig. 3 we study the behavior of the  $\lambda$ th-Rényi entropic power,  $N_\lambda[\rho_T^{(d)}] \frac{h}{k_B T}$ , as a function of the parameter  $\lambda$  for various universe dimensionalities  $d = 3 - 6$ . Briefly, we observe that (i) it monotonically decreases when  $\lambda$  is increasing for all dimensionalities, and (ii) it increases when  $d$  is increasing for all values of  $\lambda$ .

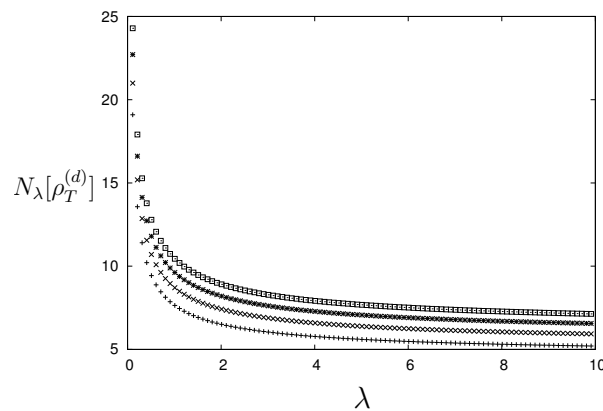


FIG. 3: Dependence of  $\lambda$ th-Rényi entropic power,  $\sigma_p[\rho_T^{(d)}]$  in  $\frac{h}{k_B T}$ -units, on the parameter  $\lambda$  for the universe dimensionalities  $d = 3(+), 4(\times), 5(*), 6(\square)$ .

### C. Biparametric Fisher information

Now we calculate the  $(p, \lambda)$ th-order Fisher information of the blackbody density  $\rho_T^{(d)}$  given by

$$\phi_{p,\lambda}[\rho_T^{(d)}] = \left( \int_{\Lambda} \left| [\rho_T^{(d)}]^{\lambda-2} \left( \rho_T^{(d)} \right)' \right|^q \rho_T^{(d)} d\nu \right)^{\frac{1}{q\lambda}}, \quad (29)$$

where  $p \in [1, \infty)$ ,  $\frac{1}{p} + \frac{1}{q} = 1$  and  $\lambda > 0$ . Operating similarly as before, we obtain that the biparametric Fisher information  $\phi_{p,\lambda}[\rho_T^{(d)}]$  of the  $d$ -dimensional blackbody density (21) at temperature  $T$  can be expressed as

$$\phi_{p,\lambda}[\rho_T^{(d)}] = [A_F(p, \lambda, d)]^{\frac{1}{q\lambda}} \frac{h}{k_B T}, \quad \forall q \in (1, \infty), \quad \forall \lambda > 0 \quad (30)$$

with the proportionality constant

$$A_F(p, \lambda, d) = \frac{I(d, q, \lambda)}{(\Gamma(d+1)\zeta(d+1))^{q\lambda-q+1}}, \quad (31)$$

where the symbol  $I(p, \lambda, d)$  denotes the integral

$$I(p, \lambda, d) = \int_{\mathbb{R}^+} \frac{x^{q(d\lambda-d-1)+d}}{(e^x-1)^{q\lambda+1}} |d(e^x-1) - xe^x|^q dx, \quad (32)$$

so that for even  $q$  and  $q\lambda \in \mathbb{N}$ , (30) one has the value

$$\begin{aligned} I(p, \lambda, d) &= \sum_{i=0}^q (-1)^{q+i} \binom{q}{i} d^i \int_0^\infty e^{(q-i)x} \frac{x^{\alpha d-i}}{(e^x-1)^{1+q\lambda-i}} dx \\ &= \sum_{i=0}^q (-1)^{q-i} \binom{q}{i} d^i (\alpha d - i)! \zeta_{\alpha+q-i}(1 + \alpha d - i, \alpha) \end{aligned}$$

with  $\alpha \equiv q\lambda - q + 1$ . Summarizing, we have obtained that the biparametric Fisher information,  $\phi_{p,\lambda}[\rho_T^{(d)}]$ , follows the law (30) with the proportionality constant

$$A_F(p, \lambda, d) = \frac{\sum_{i=0}^q (-1)^{q-i} \binom{q}{i} d^i (\alpha d - i)! \zeta_{\alpha+q-i}(1 + \alpha d - i, \alpha)}{[\Gamma(d+1)\zeta(d+1)]^\alpha} \quad (33)$$

for even  $q$  and  $q\lambda \in \mathbb{N}$ . Note that in the particular, standard case  $\lambda = 1, q = 2$ , one has that

$$A_F(2, 1, d) = \frac{1}{2\zeta(d+1)} \left( \zeta(d) - \frac{d-3}{d-1} \zeta(d-1) \right), \quad (34)$$

for  $d > 2$ . Moreover, a convergence analysis of the definition (11) allows one to show that the generalized Fisher information  $\phi_{p,\lambda}[\rho_T^{(d)}]$  given by (30) is well-defined if and only if  $\lambda p > d^* = \frac{d}{d-1}$  (which includes the condition  $\lambda > \frac{1}{1+p}$ , necessary to have finite typical deviations).

In Fig. 4 we plot a colour tridimensional map of biparametric Fisher information against its parameters  $(q, \lambda)$ , and the *conjugated* representation with respect to the parameters  $(p, \lambda)$  when  $d = 6$ . Therein we observe that biparametric Fisher information has a non-trivial behaviour with an absolute minimum valley. Similar maps can be obtained for other dimensionalities. To gain more insight into it, we make two cuts in the left colour map at  $p = 2$  and  $\lambda = 2$  obtaining the two graphs (b) at the below of the figure which show a different behavior for the corresponding generalized Fisher information. In the left graph with  $\lambda > 1/3$  a minimum shows up at  $\lambda_{min}$  for all dimensionalities  $d = 3 - 6$ . In the right graph with  $p > 1$  we observe a monotonically decreasing behavior with respect to the parameter  $p$  for all dimensionalities  $d = 3 - 6$ .

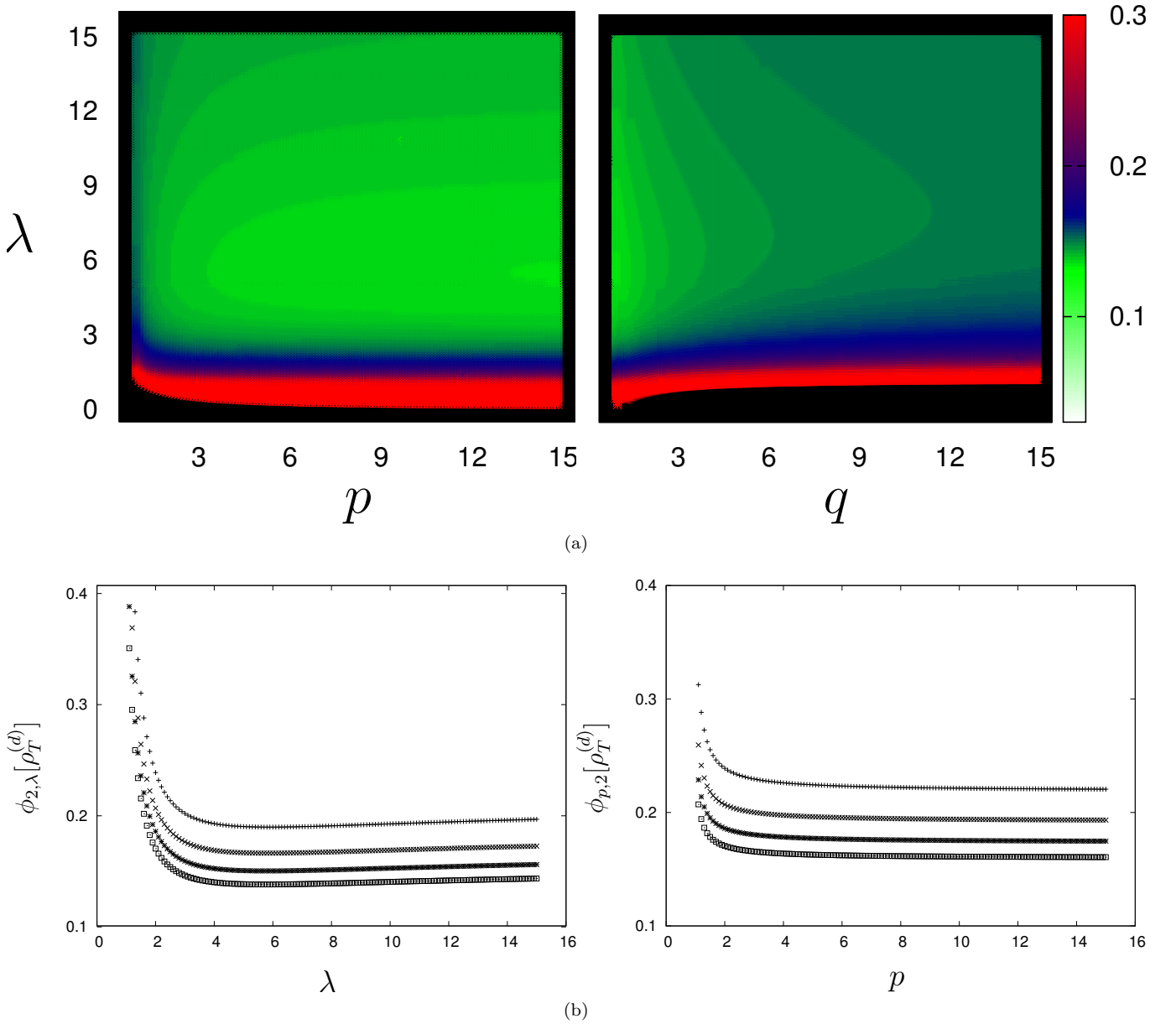


FIG. 4: Above: Colour maps of the generalized Fisher information  $\phi_{p,\lambda}[\rho_T^{(d)}]$  in  $\frac{k_B T}{h}$ -units against the parameters  $(p, \lambda)$  and  $(q, \lambda)$  respectively, when  $d = 6$ . Below left: the generalized Fisher information  $\phi_{2,\lambda}[\rho_T^{(d)}]$  in terms of  $\lambda$  for  $d = 3 - 6$ . Below right: the generalized Fisher information  $\phi_{p,2}[\rho_T^{(d)}]$  in terms of  $p$  for  $d = 3 - 6$ . In the last two graphs the upper (lower) curve corresponds to the case  $d = 3$  ( $d = 6$ ).

#### D. Biparametric complexity measures

##### 1. Biparametric Crámer-Rao complexity

Let us now calculate the generalized Crámer-Rao complexity  $C_{FR}^{(p,\lambda)}[\rho_T^{(d)}]$  of the  $d$ -dimensional blackbody density at temperature  $T$  which, according to (12), is given by

$$C_{CR}^{(p,\lambda)}[\rho_T^{(d)}] = \mathcal{K}_{CR}(p, \lambda) \phi_{p,\lambda}[\rho_T^{(d)}] \sigma_p[\rho_T^{(d)}],$$

where the constant  $\mathcal{K}_{CR}(p, \lambda)$  is given in Eq. (13). Taking into account the values of  $\phi_{p,\lambda}[\rho_T^{(d)}]$  and  $\sigma_p[\rho_T^{(d)}]$  given by Eqs. (30) and (23), respectively, we obtain that the complexity measure  $C_{FR}^{(p,\lambda)}[\rho_T^{(d)}]$  can be expressed as



$$\begin{aligned}
 C_{CR}^{(p,\lambda)}[\rho_T^{(d)}] &= \mathcal{K}_{CR}(p, \lambda) (\Gamma(d+1)\zeta(d+1))^{-\alpha} \\
 &\times \left[ \sum_{i=0}^q (-1)^{q-i} \binom{q}{i} d^i (\alpha d - i)! \zeta_{q\lambda+1-i}(1 + \alpha d - i, 1 + q(\lambda - 1)) \right]^{\frac{1}{q\lambda}} \left( \sum_{n=0}^p \gamma_n(d, p) \zeta(d+n+1) \right)^{\frac{1}{p}}, \quad (35)
 \end{aligned}$$

for even  $q$ ,  $q\lambda \in \mathbb{N}$  and where the symbol  $\gamma_n(d, p)$  is defined by (24) and  $\zeta_m(x, y)$  is the Barnes zeta function mentioned above. Most important is to note that this complexity quantifier depends only on the parameters  $(p, \lambda)$  and the dimensionality of the universe  $d$ .

In Fig. 5, we plot a colour tridimensional map of  $C_{CR}^{(p,\lambda)}[\rho_T^{(d)}] \equiv C_{CR}^{(p,\lambda)}(d)$  against the parameters  $(p, \lambda)$ , and the *conjugated* representation with respect to the parameters  $(p, \lambda)$  when  $d = 6$ . We observe that this complexity measure captures a non-trivial structure with an absolute minimum valley. Similar maps can be obtained for other dimensionalities. For completeness let us point out that when  $d = 3$ , the absolute minimum is located at  $(p \simeq 1.91, \lambda \simeq 1.55)$ , for which the complexity  $C_{CR}^{(1.91, 1.55)} \simeq 1.29$ . This illustrates to what extent the Crámer-Rao complexity captures such a structure even for distributions so well behaved as the generalized Planck distribution law. This suggests that this complexity quantifier must be a powerful tool for the information-theoretical analysis of much more complex physical laws.

To get a further insight into this complexity map  $C_{CR}^{(p,\lambda)}(d)$  we make two cuts at  $p = 2$  and  $\lambda = 2$  for various dimensionalities  $d = 3, 4, 5, 6$  as it is shown in the two below graphs of the figure. In the below-left graph we plot the complexity  $C_{CR}^{(3,\lambda)}(d)$  in terms of  $\lambda$  for  $\lambda > 1/3$ , finding the existence of a value  $\lambda_{min}$  which minimizes this measure; as well, we observe that it tends toward a constant value at large values of  $\lambda$ . In the below-right graph we plot the complexity  $C_{CR}^{(p,2)}(d)$  in terms of  $p$ , we also find a minimum but, opposite to the previous case, the asymptotic  $p$ -behavior is clearly divergent.

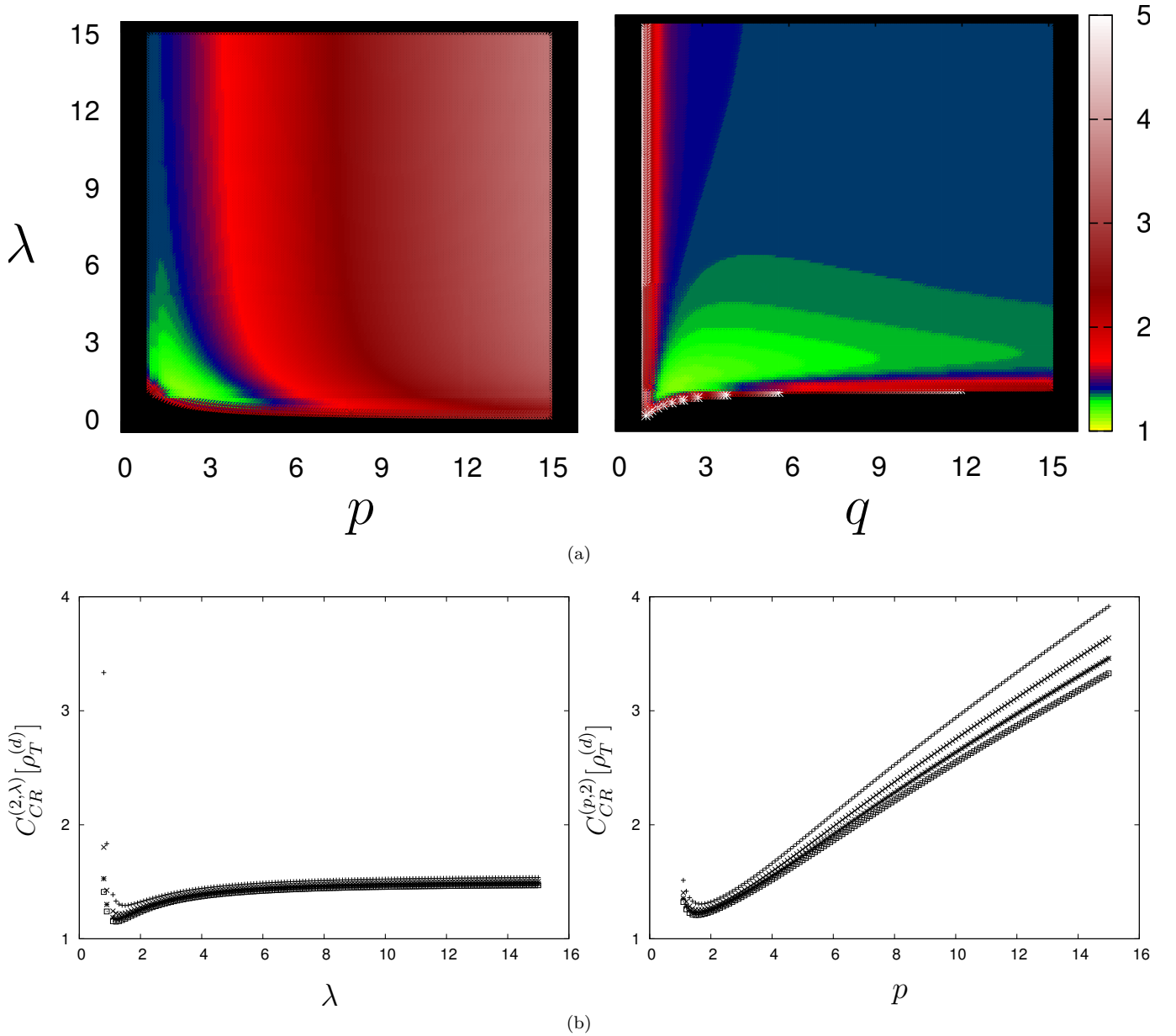


FIG. 5: Above: Colour map of the Crámer-Rao complexity  $C_{CR}^{(p,\lambda)}(d)$  against the parameters  $(p, \lambda)$  and  $(q, \lambda)$  when  $d = 6$ . Below left: Dependence of the Crámer-Rao complexity  $C_{CR}^{(2,\lambda)}(d)$  on  $\lambda$  when  $d = 6$ . Below right: Dependence of the Crámer-Rao complexity  $C_{CR}^{(p,2)}(d)$  on  $p$  when  $d = 3 - 6$ . In the last two graphs the upper (lower) curve corresponds to the case  $d = 3$  ( $d = 6$ ).

## 2. Biparametric Heisenberg-Rényi complexity

The biparametric Heisenberg-Rényi  $C_{HR}^{(p,\lambda)}[\rho_T^{(d)}]$  of the  $d$ -dimensional blackbody density  $\rho_T^{(d)}$  can be written, according to (18), as

$$C_{HR}^{(p,\lambda)}[\rho_T^{(d)}] = \mathcal{K}_{HR}(p, \lambda) \frac{\sigma_p[\rho_T^{(d)}]}{N_\lambda[\rho_T^{(d)}]}$$

with the constant  $\mathcal{K}_{HR}(p, \lambda)$  given by (19) Moreover, in the general case  $\lambda \neq 1$  this constant is

$$\mathcal{K}_{HR}(p, \lambda) = (p\lambda + \lambda - 1)^{\frac{q\lambda - \lambda + 1}{q\lambda - q}} (p\lambda)^{\frac{1}{1-\lambda}} a_{p,\lambda}^{-1},$$

so that the corresponding expression for the complexity measure  $C_{HR}^{(p,\lambda)}[\rho_T^{(d)}]$  is

$$C_{HR}^{(p,\lambda)}[\rho_T^{(d)}] = \mathcal{K}_{HR}(p, \lambda) \left( \frac{\Gamma(\lambda d + 1) \zeta_\lambda(\lambda d + 1, \lambda)}{\Gamma^\lambda(d + 1) \zeta^\lambda(d + 1)} \right)^{\frac{1}{\lambda-1}} \left( \sum_{n=0}^p \gamma_n(d, p) \zeta(d + n + 1) \right)^{\frac{1}{p}}, \quad (36)$$

with  $\lambda \in \mathbb{N}$ ,  $p$  even. Again here, we note that this complexity quantifier depends only on the parameters  $(p, \lambda)$  and the dimensionality of the universe  $d$ .

In Fig. 6, a colour tridimensional map of  $C_{HR}^{(p,\lambda)}[\rho_T^{(d)}] \equiv C_{HR}^{(p,\lambda)}(d)$  is given, which shows the dependence of the Heisenberg-Rényi complexity in terms of the parameter  $\lambda$  for different values of the parameter  $p$  for the spatial dimensionality  $d = 6$ . We observe that Heisenberg-Rényi complexity measure allows us to capture a non-trivial structure with an absolute minimum. Similar complexity maps can be obtained for other dimensionalities. In particular when  $d = 3$  this minimum is located at  $(p \simeq 1.34, \lambda \simeq 1.24)$ , for which this measure has the value  $C_{CR}^{(1.34, 1.24)} \simeq 1.08$ . To better understand this figure at the dimensionalities  $d = 3, 4, 5, 6$ , we make two cuts at  $p = 3$  and at  $\lambda = 1$  which give rise to the two below graphs. In the below-left graph we plot the complexity  $C_{HR}^{(3,\lambda)}(d)$  in terms of  $\lambda$  for  $\lambda > 1/4$ , finding the existence of a  $\lambda_{min}$  which minimizes the measure as well as a constant asymptotic trend when  $\lambda \rightarrow \infty$ . In the below-right graph we plot the complexity quantifier  $C_{HR}^{(p,1)}(d)$  for  $p > 0$ , finding a minimum value  $p_{min}$  which minimizes the complexity, as well as a divergent asymptotic behavior similar to the one previously found for the Crámer-Rao complexity measure.

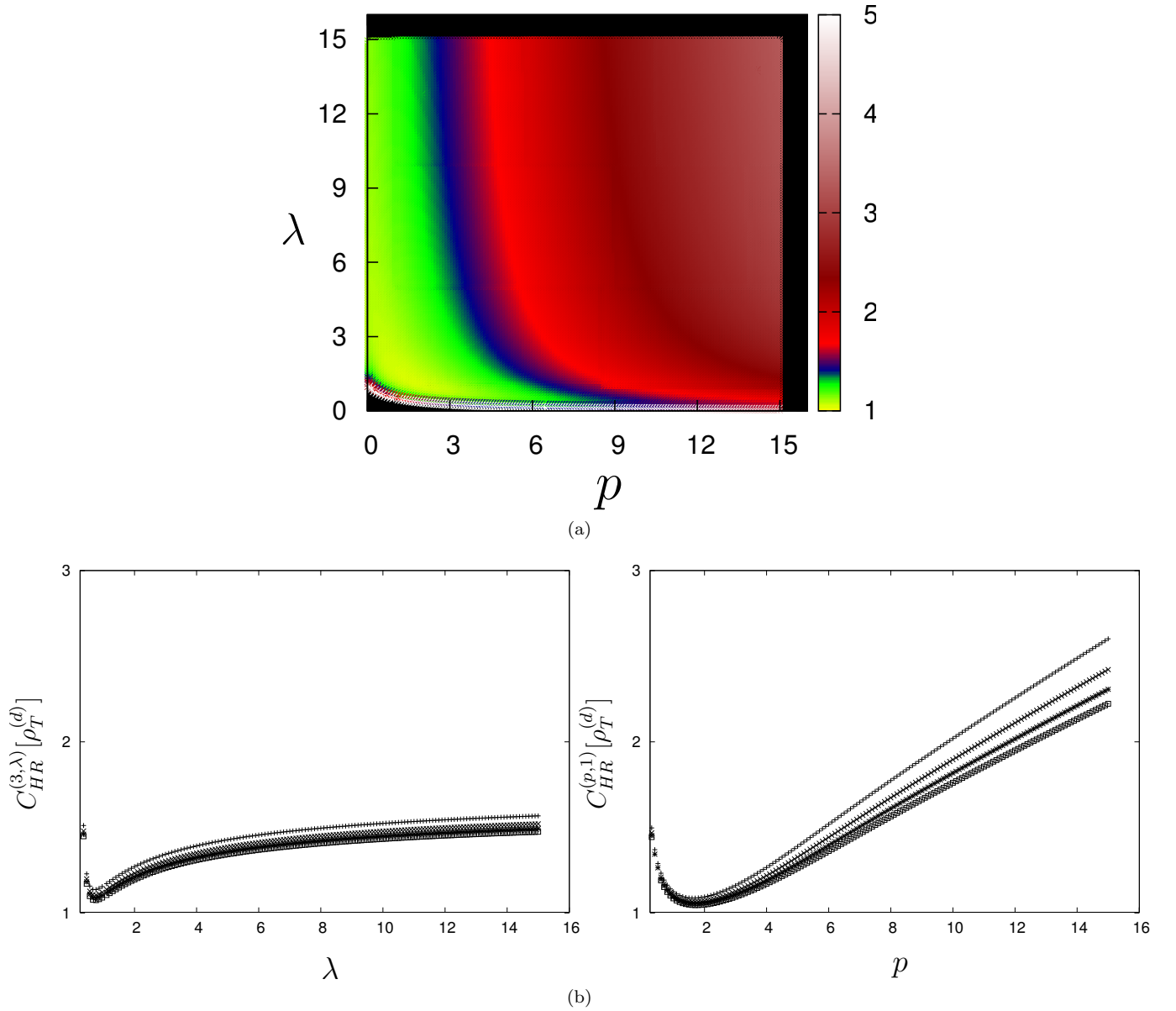


FIG. 6: Above: Colour map of the Heisenberg-Rényi complexity  $C_{HR}^{(p,\lambda)}[\rho_T^{(d)}] \equiv C_{HR}^{(p,\lambda)}(d)$  against the parameters  $(p, \lambda)$  when  $d = 6$ . Below left: Dependence of the Heisenberg-Rényi complexity  $C_{HR}^{(3,\lambda)}(d)$  on  $\lambda$  when  $d = 3 - 6$ . Below right: Dependence of the Heisenberg-Rényi complexity  $C_{HR}^{(p,1)}(d)$  on  $p$  when  $d = 3 - 6$ . In the last two graphs the upper (lower) curve corresponds to the case  $d = 3$  ( $d = 6$ ).

Finally, for completeness, in Fig. 7 the generalized Gaussian distributions which minimize the two novel complexity quantifiers of Crámer-Rao (red color) and Heisenberg-Rényi (blue) types introduced in this work are compared with the corresponding Planck distribution law (black) for the dimensionality  $d = 3$ . We observe certain similarities in the left fall of the Crámer-Rao and Planck cases, and in the right fall of the Heisenberg-Rényi and Planck cases.

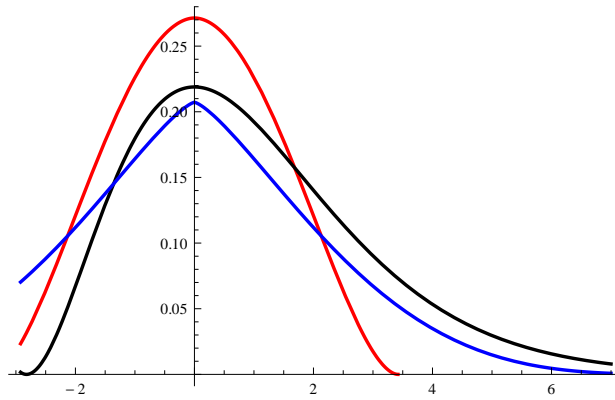


FIG. 7: Comparison of the generalized Gaussian minimizers of the extended Crámer-Rao (red) and Heisenberg-Rényi (blue) with Plank distribution law (black) when  $d = 3$ .

#### IV. CONCLUSIONS AND OPEN PROBLEMS

It is known that we need various measures to take into account the multiple facets of the concept of complexity in a complex many-body system. In this paper we have introduced and discussed two novel biparametric complexity tools of Crámer-Rao and Heisenberg-Rényi types, which extend the three basic measures of complexity (i.e., Crámer-Rao, Fisher-Shannon and LMC) and some modifications which have been published up until now. Then we have illustrated the usefulness of these two complexity measures by applying and explicitly computing them for a relevant quantum object, the  $d$ -dimensional blackbody at temperature  $T$ . We have found that they are universal constants in the sense that they are dimensionless and they do not depend on the temperature nor on any physical constant (such as e.g., Planck constant, speed of light or Boltzmann constant), so that they only depend on the spatial dimensionality of the universe. The results show the existence of a non trivial underlying mathematical structure, according to which these quantities become minimal for some values of their characteristic parameters.

To determine these generalized measures of complexity for the  $d$ -dimensional blackbody radiation with standard ( $d = 3$ ) and non-standard dimensionalities we needed to calculate various dispersion and entropy-like quantities in terms of dimensionality  $d$  and temperature  $T$ . Indeed, we have determined the typical deviations (that generalize the standard deviation), the Rényi entropy (that generalizes the Shannon entropy and the disequilibrium) and the biparametric Fisher information (which generalizes the standard Fisher information) of the  $d$ -dimensional Planck density in an analytical way. We have found that these quantities, slightly modified, have a Wien-like temperature behavior similar to the well-known Wien's law followed by the frequency  $\nu_{max}$  at which the density is maximum. The values of these characteristic quantities, particularly the ones associated to the biparametric Fisher information, might be of potential interest to grasp the anisotropies of the cosmic microwave background radiation (which yields information about our Universe at around 380 000 years after the Big Bang). Finally, we wonder whether this information-theoretical approach may be used for the (broadly unknown) cosmic neutrino background and the cosmic gravitational background, which would provide hints about our Universe one minute after the Big Bang and during the Big Bang, respectively [72].

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Statement: All authors contributed equally to the paper.

## V. APPENDIX A

Here we explicitly solve the integral functionals needed to determine the Rényi entropies of the  $d$ -dimensional blackbody in section III.

**Lemma.** Let  $n, m, k \in \mathbb{N}_0, n, k > 0, n > k \geq m$  y  $r, s, p \in \mathbb{R}$ , con  $r > s, r > p$ . Then, the following multiparametric integral has the value

$$\begin{aligned} \int_0^\infty \frac{x^n e^{(mr+(k-m)s+p)x}}{(e^{rx} - e^{sx})^{k+1}} dx &= \frac{1}{(r-s)^{n+1}} \frac{n!}{k!} \sum_{i=0}^k \sum_{j=0}^{k-i} (-1)^{k+i} \binom{i+j}{j} S_k^{(i+j)} \left( k-m + \frac{s-p}{r-s} \right)^j \zeta \left( n+1-i, \frac{r-p}{r-s} \right) \\ &= \frac{1}{(r-s)^{n+1}} n! \sum_{i=0}^k q_{k+1,i} \left( k-m + \frac{r-p}{r-s} \right) \zeta \left( n+1-i, \frac{r-p}{r-s} \right), \end{aligned} \quad (37)$$

where the Stirling numbers  $S_n^{(l)}$  and the Choi coefficients are related by Eq. (28).

*Proof.* Let us begin with the multiparametric functional

$${}_k^t J_m^n(r, s, p) = \int_0^\infty \frac{x^n e^{(m-k)rx} e^{(m-t)sx} e^{px}}{(e^{rx} - e^{sx})^m} dx \quad (38)$$

with  $r > 0, r > s, r > p$ , y  $n, m, k, t \in \mathbb{N}, n+1 > m \geq k, t$ . By deriving this functional with respect to  $s$  and  $r$ , one readily finds some recurrence relations  ${}_k^t J_m^n(r, s, p)$  for it. For convenience, however, we first make the change of variable  $y = (r-s)x$ , because then one realizes that the functional only depends on  $\frac{r-p}{r-s}$  when  $m+1 = k+t$ , so that it is better to write

$${}_k^t J_{k+t-1}^n(r, s, p) = \frac{1}{(r-s)^{n+1}} {}_k^t f_{k+t-1}^n \left( \frac{r-p}{r-s} \right), \quad (39)$$

and then the abovementioned derivations yield the following recurrence relations:

$${}_k^1 f_{k+1}^{n+1}(x) = \frac{1}{k} \left[ \left( n+1 + x \frac{d}{dx} \right) {}_k^1 f_k^n(x) - (k-1) {}_k^1 f_k^{n+1}(x) \right] \quad (40)$$

$${}_k^{t+1} f_{k+t}^{n+1}(x) = \frac{1}{k+t-1} \left[ \left( n+1 + (x-1) \frac{d}{dx} \right) {}_k^t f_{k+t-1}^n(x) + (t-1) {}_k^t f_{k+t-1}^{n+1}(x) \right]. \quad (41)$$

On the other hand we can obtain that

$${}_1^1 f_1^n(r, s, p) = (-1)^{n+1} \psi^{(n)} \left( \frac{r-p}{r-s} \right), \quad (42)$$

by noticing that  ${}_1^1 J_1^n(r, s, p)$  is the  $n$ -th derivative of the integral (see Eq. 3.311-11 of Ref. [73])

$$\int_0^\infty \frac{e^{px} - e^{qx}}{e^{rx} - e^{sx}} dx = \frac{1}{r-s} \left[ \psi \left( \frac{r-q}{r-s} \right) - \psi \left( \frac{r-p}{r-s} \right) \right],$$

with respect to  $p$ . The symbol  $\psi^{(n)}(x)$  denotes the  $n$ th derivative of the digamma function [69].

The recurrence relation (40) with the initial condition (42) gives rise by induction to

$${}_k^1 f_k^n(x) = \frac{(-1)^{k+n}}{(k-1)!} \sum_{j=0}^{k-1} \sum_{i=0}^{k-j-1} \binom{n}{j} \frac{(i+j)!}{i!} S_{k-1}^{(i+j)} (x+k-2)^i \psi^{(n-j)}(x). \quad (43)$$

Then, the recurrence relation (43) in  $t$  with the initial ( $t=0$ ) condition allows us to obtain also by induction the expression

$${}_k^{t+1} f_{k+t}^n(x) = \frac{(-1)^{k+t+n}}{(k+t-1)!} \sum_{j=0}^{k+t-1} \sum_{i=0}^{k+t-j-1} \binom{n}{j} S_{k+t-1}^{(i+j)} \frac{(i+j)!}{i!} (x+k-2)^i \psi^{(n-j)}(x). \quad (44)$$

Now the replacement of (44) into (39), taking into account that  $\psi^{(n)}(x) = (-1)^{n+1}n!\zeta(n+1, x)$  and redefining the involved parameters in a convenient manner, we finally obtain the wanted expression (37):

$$\int_0^\infty \frac{x^n e^{mrx} e^{(k-m)sx} e^{px}}{(e^{rx} - e^{sx})^{k+1}} dx = \frac{1}{(r-s)^{n+1}} \frac{n!}{k!} \sum_{i=0}^k \sum_{j=0}^{k-i} (-1)^{k+i} \binom{i+j}{j} S_k^{(i+j)} \left(k - m + \frac{s-p}{r-s}\right)^j \zeta\left(n+1-i, \frac{r-p}{r-s}\right)$$

where  $n, m, k \in \mathbb{N}$ ,  $n > k \geq m$  y  $r, s, p \in \mathbb{R}$ , con  $r > s, r > p$ . And from this expression and Eq. (28) follows the second expression of the Lemma. □

**Corollary.** *Let  $k \in \mathbb{N}$ ,  $a \in \mathbb{R}$ ,  $n \in \mathbb{N}$ . Then, the following finite sum of standard Hurwitz functions  $\zeta(s, a)$*

$$Z_k(n, a, t) = \sum_{i=0}^{k-1} q_{k,i}(a) \zeta(n-i, t), \tag{45}$$

verifies

$$\zeta_k(n, a) = Z_k(n, a, \{a\}) = Z_k(n, a, 1 + \{a\}) = \dots = Z_k(n, a, a), \tag{46}$$

$\forall a \in \mathbb{R}/\mathbb{N}$  (with  $\{a\} \equiv a - [a]$  being the non-integer part of  $a$ ), and

$$\zeta_k(n, a) = Z_k(n, a, 1) = Z_k(n, a, 2) = \dots = Z_k(n, a, a), \quad \forall a \in \mathbb{N}. \tag{47}$$

*Proof.* Using the previous Lemma with  $s = 0$ ,  $r = 1$  and  $p < 1$  for  $k, m, n \in \mathbb{N}_0$  and  $n > k \geq m$  one has that

$$\frac{1}{n!} \int_0^\infty \frac{x^n e^{(m+p)x}}{(e^x - 1)^{k+1}} dx = \sum_{i=0}^k q_{k+1,i}(k-m-p+1) \zeta(n+1-i, 1-p). \tag{48}$$

On the other hand, taking into account the integral representation [70] with  $m+p = k+1-a$  we can write

$$\zeta_{k+1}(n+1, a) = \frac{1}{\Gamma(n+1)} \int_0^\infty \frac{x^n e^{(m+p)x}}{(e^x - 1)^{k+1}} dx = \sum_{i=0}^k q_{k+1,i}(a) \zeta(n+1-i, 1-p) \tag{49}$$

(where the last identity holds provided that  $1 > p = k+1-m-a \geq 1-a$ ) and using the notation  $a - [a] \equiv \{a\}$ , where  $[a]$  denotes the integer part of  $a \in \mathbb{R}$ , it is straightforward to see that  $p + \{a\} = k+1-m-[a] \equiv n' \in \mathbb{N}$ . The latter implies that, due to the conditions  $0 \leq m \leq k$  and  $p < 1$ , the values of  $p$  are limited to  $p = 1-a, 2-a, \dots, [a]+1-a < 1$ ,  $\forall a \in \mathbb{R}/\mathbb{N}$ ; for  $a \in \mathbb{N}$  the inequality is fulfilled for  $p = 1-a, \dots, [a]-a = 0 < 1$ . Thus, we have proved that

$$\zeta_{k+1}(n+1, a) = \sum_{i=0}^k q_{k+1,i}(a) \zeta(n+1-i, 1-p)$$

where  $p$  can take the values  $p = 1-a, 2-a, \dots, 1-\{a\}$ , save when  $a \in \mathbb{N}$  in which case  $p = 1-a, 2-a, \dots, 0$  so that then one has

$$\zeta_k(n, a) = Z_k(n, a, \{a\}) = Z_k(n, a, 1 + \{a\}) = Z_k(n, a, 2 + \{a\}) = \dots = Z_k(n, a, a) \tag{50}$$

$\forall a \in \mathbb{R}/\mathbb{N}$ , and

$$\zeta_k(n, a) = Z_k(n, a, 1) = Z_k(n, a, 2) = \dots = Z_k(n, a, a) \quad \forall a \in \mathbb{N}. \tag{51}$$

□

**Corollary.** *For  $k \in \mathbb{N}$ ,  $n \in \mathbb{N}$ ,  $m \in \mathbb{N}_0$ , and  $n+1 > k > m \geq 0$  one has that*

$$\frac{1}{n!} \int_0^\infty \frac{x^n e^{mx}}{(e^x - 1)^k} dx = \sum_{i=0}^{k-1} q_{k,i}(k-m) \zeta(n+1-i).$$

This result directly follows from the previous Lemma with  $r = 1$  and  $s = p = 0$ .

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## Chapter 6

# Differential-escort transformations and the LMC-Rényi complexity

In this chapter we introduce the notion of differential-escort transformation  $\mathfrak{E}_\alpha$  of a probability density  $\rho(x)$ , we discuss its most important properties and then we illustrate its usefulness (i) by applying it to the exponential and power-law decaying densities and (ii) by proving the unknown monotonicity property of the LMC-Rényi complexity measure. Basically, a differential-escort transformation is similar to a escort one, but the normalization process is done through a non-linear variable change. Let us advance that the proof of the monotonicity of the LMC-Rényi complexity basically rests in the convexity behaviour of the Rényi entropy of a differential-escort density with respect to the transformation parameter  $\alpha$ , which in turn is proven by means of Jensen's inequality. Moreover, the control over this property of monotonicity allows us to explore the entropic behaviour in the low and high complexity limits. Finally, the q-exponential Tsallis' densities are obtained as the differential-escort transformation of the exponential one, what is an illustration of the capability of these transformations to dramatically change the tail of the distribution.

Specifically, we have carried out the following tasks:

- We define the notion of differential-escort transformation  $\mathfrak{E}_\alpha$  of the probability density  $\rho$ . We will call by differential-escort density,  $\rho_\alpha$ , to the differential-escort-transformed of  $\rho$ ; that is,  $\rho_\alpha \equiv \mathfrak{E}_\alpha[\rho]$ .
- We prove and discuss the basic mathematical properties of these transformations. Here let us just advance its composition law

$$\mathfrak{E}_\alpha[\mathfrak{E}_{\alpha'}[\rho]] = \mathfrak{E}_{\alpha'}[\mathfrak{E}_\alpha[\rho]] = \mathfrak{E}_{\alpha\alpha'}[\rho]$$

- We find the following linear law for the Shannon entropy of the differential-escort density  $\rho_\alpha$ , as well as, a pseudo-linear law for the Rényi and Tsallis entropy through a rescaling of the entropic parameter:

$$\frac{S[\rho_\alpha]}{S[\rho]} = \frac{R_\lambda[\rho_\alpha]}{R_{\lambda_\alpha}[\rho]} = \frac{T_\lambda[\rho_\alpha]}{T_{\lambda_\alpha}[\rho]} = \alpha, \quad \lambda_\alpha = 1 + \alpha(\lambda - 1).$$

- We prove the convexity of the Rényi entropy  $R_\lambda$  of the differential-escort density  $\rho_\alpha$  on the transformation parameter  $\alpha$ , which depends on the sign of  $\lambda - 1$  as

$$\text{sgn} \left( \frac{\partial^2 R_\lambda[\rho_\alpha]}{\partial \alpha^2} \right) = \text{sgn}(1 - \lambda).$$

- We prove the monotonicity behaviour of the LMC-Rényi complexity measure with respect to the differential-escort transformation:

$$C_{\lambda,\beta}[\rho_{\alpha'}] \geq C_{\lambda,\beta}[\rho_\alpha], \quad \alpha' > \alpha > 0.$$

In particular, the following result is obtained: Given the family of uniform distributions  $\Xi$ , and the class of transformations  $\mathfrak{E}_\alpha$ , then the triplet  $(C_{\lambda,\beta}, \Xi, \mathfrak{E}_\alpha)$  satisfies the monotonicity property of the LMC-Rényi measure of complexity.

- We study the entropic and complexity behaviour of a differential-escort density  $\rho_\alpha$  when it is strongly deformed to the *low complexity limit* ( $\alpha \rightarrow 0$ ) and to the *high complexity limit* ( $\alpha \rightarrow \infty$ ).
- We apply the differential-escort transformation to the exponential and power-law decaying densities. We find, in particular, that the full family of q-exponential densities can be obtained as the differential-escort transformations of the exponential density.

These results are contained in the preprint [71] with coordinates: **Puertas-Centeno D.** *Differential escort distributions and LMC-Rényi complexity monotonies*, preprint UGR 2018, which is attached below.

# Differential-escort transformations and the LMC-Rényi complexity measure

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Escort distributions have been shown to be very useful in a great variety of fields ranging from information theory, nonextensive statistical mechanics till coding theory, chaos and multifractals. In this work we give the notion and the properties of a novel type of escort density, the *differential escort densities*, which have various advantages with respect to the standard ones. We highlight the behaviour of the Shannon, Rényi and Tsallis entropies of these distributions. Then, we illustrate their utility to prove the monotonicity property of the LMC-Rényi complexity measure and to study the behaviour of general distributions in the two extreme cases of minimal and very high LMC-Rényi complexity. Finally, this transformation allows us to obtain the Tsallis  $q$ -exponential densities as the differential escort transformation of the exponential density.

## 1 Introduction

The study of chaotic and complex systems have needed the development of mathematical tools able to capture the fundamental statistical properties of the system. Escort distributions have been introduced in statistical physics for the characterization of multifractals systems [1]. These distributions  $\{\tilde{p}_i\}$  conform a one-parameter class of transformations of an original probability distribution  $\{p_i\}$  according to  $\tilde{p}_i = \frac{p_i^q}{\sum_{i=1}^N p_i^q}$ . with  $q \in \mathbb{R}$ .

This idea previously appeared in relation to the Rényi-entropy-based coding theorem [2, 3] and Rényi-entropy-based fractal dimensions [4]. The mathematical properties of the discrete escort distributions have been widely studied [5, 6, 7, 8]. This concept can be easily extended to the continuous case. Given a real variable  $x \in \mathbb{R}$  and a probability distribution  $\rho(x)$ , such that

$\int_{\mathbb{R}} \rho(x) dx = 1$ , one has the escort distribution [9] defined as

$$E_q[\rho](x) \equiv \tilde{\rho}(x) = \frac{[\rho(x)]^q}{\int_{\mathbb{R}} [\rho(t)]^q dt} \quad (1)$$

on the assumption that  $\int_{\mathbb{R}} \rho(x)^q dx < \infty$ . Note that the parameter  $q$  plays a focus role to highlight different regions of  $\rho(x)$ . These distributions play a relevant role in coding problems, non-equilibrium statistical mechanics [10, 11] and electronic structure [12, 13, 14]. A particular example is the  $q$ -exponential distribution

$$e_q(x) \propto (1 + (q - 1)|x|)^{\frac{1}{1-q}} \quad (2)$$

which maximizes the Rényi entropy

$$R_q[\rho] = \frac{1}{1 - q} \log \left( \int_{\mathbb{R}} [\rho(x)]^q dx \right) \quad (3)$$

and the Tsallis entropy

$$T_q[\rho] = \frac{1}{1 - q} \left( 1 - \int_{\mathbb{R}} [\rho(x)]^q dx \right) \quad (4)$$

subject to average-constraints governed by its escort distribution. Of course, in the limit  $q \rightarrow 1$  the original distribution is recovered in Eq. (1), the exponential distribution is also recovered in Eq. (2) and the Shannon entropy

$$S[\rho] = \lim_{q \rightarrow 1} R_q[\rho] = \lim_{q \rightarrow 1} T_q[\rho] = - \int_{\mathbb{R}} \rho(t) \log[\rho(t)] dt \quad (5)$$

is respectively recovered in Eqs (3) and (4).

The aim of this work is to introduce the notion of *differential-escort transformation*,  $\mathfrak{E}_\alpha$ , and to study its basic mathematical properties (probability invariance, composition rule, scaling property,...). Then, we highlight the strongly regular behaviour of the Shannon, Rényi and Tsallis entropies under this transformation, observing that the entropic parameter naturally rescales similarly to the rescaling behavior recently found by Korbel [15] for the non-additivity parameter in Tsallis thermostatics [16]. This behavior is related to the rescaling of the relative fluctuations of a system with a finite number of particles, and plays a relevant role in the deformed calculus developed by Borges [17] as it is discussed by Korbel himself. Moreover we also note that the  $q$ -exponential distribution is just the differential-escort transformation of the standard exponential distribution; so, differently to what happens to the

the standard escort transformation of an exponential distribution which is another exponential. In fact, we show that the differential-escort transformation changes the behaviour of the distribution tail in a deeper and more interesting manner than the standard escort transformation. Finally, the notion of *differential escort density* allows us to solve the monotonicity problem of the LMC-Rényi complexity measure [18, 19] recently posed by Rudnicki et al [20], as well as to propose a possible characterization of power-law-decaying probability densities through Lemma 1.

The structure of this work is the following: In section 2 the differential-escort transformation  $\mathfrak{E}_\alpha$  is defined and its basic mathematical properties are given. In section 3 the entropic properties of the differential escort densities are discussed. In section 4 the LMC-Rényi complexity of the differential escort densities is studied and the monotonicity property of this measure is proven. In section 5 the entropic and complexity behaviour of a general probability density when it is deformed until to the low and high complexity limits is studied. Then, in section 6 this transformation is applied to distributions of exponential, q-exponential and general power-law decaying distributions. Finally, in section 7 some conclusions and open problems are given.

## 2 Differential-escort transformation

In this section we give the notion and properties of the differential escort transformation. Let us advance that the basic difference with the standard escort transformations is the normalization process. Indeed, while an escort density is normalized according to (1), in the differential-escort case the normalization is achieved through a variable change which imposes the conservation of the probability in any differential interval of the support, as we will see later.

### The notion

Let us consider a probability density  $\rho(x), x \in \Lambda \subseteq \mathbb{R}$ , normalized, so that  $\int_\Lambda \rho(x)dx = 1$ ; and let us denote  $\mathcal{D}(\mathbb{R})$  for the set of any distribution  $\rho$  on any subset of  $\mathbb{R}$ .

**Definition 1.** *Let  $\alpha \in \mathbb{R}$ , and  $\rho \in \mathcal{D}(\mathbb{R})$  a probability density with a connected support<sup>1</sup>  $\Lambda$ , we define the transformation  $\mathfrak{E}_\alpha : \mathcal{D}(\mathbb{R}) \longrightarrow \mathcal{D}(\mathbb{R})$  as:*

---

<sup>1</sup>We assume that the support is connected for easier reading. The definition could be easily extended to any distribution without disturbing its properties.

$$\mathfrak{E}_\alpha[\rho](y) \equiv [\rho(x(y))]^\alpha \quad (6)$$

where  $y = y(x)$  is a bijection defined by:

$$\frac{dy}{dx} = [\rho(x)]^{1-\alpha}, \quad y(x_0) = x_0, \quad x_0 \in \Lambda \quad (7)$$

The support  $\Lambda_\alpha$  of the transformed density  $\mathfrak{E}_\alpha[\rho]$  is given as  $\Lambda_\alpha = y(\Lambda) = \{y \in \mathbb{R} \mid y = y(x), x \in \Lambda\}$ . To make a easier reading we will denote  $\rho_\alpha(y) \equiv \mathfrak{E}_\alpha[\rho](y)$ , and generally we will take  $x_0 = 0$ , and  $y(x) = \int_0^x [\rho(t)]^{1-\alpha} dt$ .

We remark that this definition is valid for any  $\alpha \in \mathbb{R}$ , contrary with the standard escort distribution for which the parameter  $q$  is restricted by the condition  $\int_\Lambda [\rho(x)]^\alpha dx < \infty$  as already indicated in Eq. (1). This extension is possible since the support of a differential-escort density  $\Lambda_\alpha$  does not remain invariant contrary to the standard escort case. As we will see later, for any probability density  $\rho$ , the operation (1) defines a transformed density  $\rho_\alpha$  for any  $\alpha \in \mathbb{R}$ .

Let us also point out that the election of  $x_0$  only implies a translation. In addition, when  $\alpha = 1$ , one has that the operation  $\mathfrak{E}_\alpha$  corresponds to the identity, i.e.,  $\mathfrak{E}_1[\rho] = \rho$ ; and when  $\alpha = 0$ , the operation  $\mathfrak{E}_\alpha$  transform  $\rho$  to an uniform distribution with an unitary support, concretely

$$\mathfrak{E}_0[\rho](x) = \begin{cases} 1, & x \in [x_0 - p_-, x_0 + p_+] \\ 0, & \text{otherwise} \end{cases},$$

where  $p_- = Prob[x < x_0]$  and  $p_+ = Prob[x > x_0]$ .

## The basic properties

In the following we will give some basic properties of the differential-escort transformation.

Property 1 is the most characteristic property of this transformation which consists in a strong probability invariance far beyond the mere conservation of the norm of the *standard escort* case.

### Property 1. *Probability invariance*

Let  $\alpha \in \mathbb{R}$  and  $\rho$  a probability density with a connected support  $\Lambda$ . Then, for any pair of points  $x_1, x_2 \in \Lambda$  and respectively  $y_1 = y(x_1)$  and  $y_2 = y(x_2)$  the identity

$$\int_{x_1}^{x_2} \rho(x) dx = \int_{y_1}^{y_2} \rho_\alpha(y) dy, \quad (8)$$

or equivalently

$$\text{Prob}[x \in [x_1, x_2]] = \text{Prob}[y \in [y_1, y_2]], \quad (9)$$

is fulfilled.

*Proof.* This property follows straightforwardly from (1) since

$$\int_{y_1}^{y_2} \rho_\alpha(y) dy = \int_{x_1}^{x_2} [\rho(x)]^\alpha \frac{dy}{dx} dx = \int_{x_1}^{x_2} [\rho(x)]^\alpha [\rho(x)]^{1-\alpha} dx = \int_{x_1}^{x_2} \rho(x) dx$$

□

This property makes a deep difference with escort distributions. While for the latter ones the conservation of the norm is imposed dividing by a real number as indicated in (1), for the differential-escort distributions it naturally holds as a consequence of property 1 since  $\int_{\Lambda_\alpha} \rho_\alpha(y) dy = \int_{\Lambda} \rho(x) dx = 1$ . Moreover, a similar property is fulfilled by a relevant transformation between auxiliary and physical probability densities in the context of quantum gravity [21].

**Property 2. Composition law**

Let the real numbers  $\alpha, \alpha'$ , then

$$\mathfrak{E}_\alpha[\mathfrak{E}_{\alpha'}[\rho]] = \mathfrak{E}_{\alpha'}[\mathfrak{E}_\alpha[\rho]] = \mathfrak{E}_{\alpha\alpha'}[\rho] \quad (10)$$

holds.

*Proof.* By definition,  $\mathfrak{E}_\alpha[\rho(x)](y) \equiv \rho_\alpha(y) = [\rho(x)]^\alpha$ , where  $dy = [\rho(x)]^{1-\alpha} dx$ . Moreover, one has  $\mathfrak{E}_\gamma[\mathfrak{E}_\alpha[\rho(x)]](z) = \mathfrak{E}_\gamma[\rho_\alpha(y)](z) = [\rho_\alpha(y)]^\gamma = [\rho(x)]^{\alpha\gamma}$  where  $dz = [\rho_\alpha(y)]^{1-\gamma} dy$ , so that one has  $dz = [\rho(x)]^{\alpha(1-\gamma)} [\rho(x)]^{1-\alpha} dx = [\rho(x)]^{1-\alpha\gamma} dx$ . □

This property is similar to the one of the standard escort transformations, but the latter one holds in a more restrictive sense by taking into account that the standard escort transformations are not typically well defined for any  $\alpha \in \mathbb{R}$ . On the other hand this property allows us to find the inverse element of the differential-escort transformation

$$[\mathfrak{E}_\alpha]^{-1} = \mathfrak{E}_{\alpha^{-1}}, \quad \alpha \neq 0, \quad (11)$$

what allows us to say that  $\mathfrak{E}_{\alpha \neq 0}[\mathcal{D}(\mathbb{R})] = \mathcal{D}(\mathbb{R})$ .

Let us finally give the composition rule between the differential-escort and the scaling transformations. For example, in the standard escort case,  $\tilde{\rho}$ , defined in Eq. (1) the composition rule with the scaling transformation is given by  $E_\alpha[\rho^{(a)}] = E_\alpha[\rho]^{(a)}$ , where  $\rho^{(a)}$  denotes the scaling transformed distribution  $\rho^{(a)}(x) = a\rho(ax), a > 0$ . As stated in the following property the composition law for the differential-escort case the power operation is inherited by the scaling parameter  $a$ .



**Property 3. *Scaling Property***

Let  $a \in \mathbb{R}_+$ ,  $\alpha \in \mathbb{R}$ ,  $\rho$  a probability distribution, and the scaling transformed distribution  $\rho^{(a)}(x) = a\rho(ax)$ . Then, it holds

$$\mathfrak{E}_\alpha[\rho^{(a)}] = \mathfrak{E}_\alpha[\rho]^{(a^\alpha)} \quad (12)$$

*Proof.* From the hypotheses of this statement one has the associated differential-escort distribution  $\rho_\alpha(y) = \rho(x)^\alpha$ , where  $y(x) = \int_0^x [\rho(t)]^{1-\alpha} dt$ , or equivalently  $y = \int_0^{x(y)} [\rho(t)]^{1-\alpha} dt$ . Later, we consider the differential-escort distribution of the scaling transformed: we obtain  $(\rho^{(a)})_\alpha(z) = [\rho^{(a)}(x)]^\alpha$ , with  $z(x) = \int_0^x [\rho^{(a)}(t)]^{1-\alpha} dt$ , so we have :

$$(\rho^{(a)})_\alpha(z) = a^\alpha [\rho(ax(z))]^\alpha, \quad z(x) = a^{-\alpha} \int_0^{ax} [\rho(t)]^{1-\alpha} dt$$

Then, we can write  $a^\alpha z = \int_0^{ax(z)} [\rho(t)]^{1-\alpha} dt$ . On the other hand, taking into account that  $y = \int_0^{x(y)} [\rho(t)]^{1-\alpha} dt$ , we have that  $ax(z) = x(a^\alpha z)$  and finally

$$(\rho^{(a)})_\alpha(z) = a^\alpha [\rho(x(a^\alpha z))]^\alpha = a^\alpha \rho_\alpha(a^\alpha z) = \rho_\alpha^{(a^\alpha)}(z).$$

□

### 3 The entropic properties

The functional ingredients of Rényi and Tsallis entropies (3), (4) are the entropic moments of the probability distribution  $\rho$

$$W_q[\rho] = \int_{\mathbb{R}} [\rho(x)]^q dx \quad (13)$$

In this section we will study the behaviour of these entropy-like functionals for the differential-escort distributions, finding that it is much simpler than the corresponding one for the standard escort case. Interestingly, the rescaling

$$q_\alpha = 1 + \alpha(q - 1), \quad (14)$$

for the parameter  $q$ , so much relevant in deformed algebra [17] and Tsallis thermostatics [15], naturally appears in the entropic moment  $W_q$  of the differential-escort distributions as shown in the next property.

**Property 4. *Rescaling of the entropic moments***

Let  $\rho$  be a probability distribution,  $a \in \mathbb{R}$  and  $\alpha \in \mathbb{R}$ . Then the entropic moments  $W_q[\rho]$  transform as

$$W_q[\rho_\alpha] = W_{q_\alpha}[\rho], \quad (15)$$

where  $q_\alpha$  is given in (14).

*Proof.* If  $W_q[\rho_\alpha] < \infty$ , then

$$W_q[\rho_\alpha] = \int_{\mathbb{R}} [\rho_\alpha(y)]^q dy = \int_{\mathbb{R}} [\rho(x)]^{\alpha q} [\rho(x)]^{1-\alpha} dx = W_{1+(q-1)\alpha}[\rho]$$

In case that  $W_q[\rho_\alpha] = \infty$ , we consider the following equality between finite integrals

$$\int_{y_1}^{y_2} [\rho_\alpha(y)]^q dy = \int_{x_1}^{x_2} [\rho(x)]^{q\alpha} dx$$

for any  $x_1, x_2 \in \Lambda$  and  $y_{1,2} = y(x_{1,2})$ . So, one has

$$\frac{W_q[\rho_\alpha]}{W_{q\alpha}[\rho]} = \lim_{(x_1, x_2) \rightarrow (x_m, x_M)} \frac{\int_{y_1}^{y_2} [\rho_\alpha(y)]^q dy}{\int_{x_1}^{x_2} [\rho(x)]^{q\alpha} dx} = \lim_{(x_1, x_2) \rightarrow (x_m, x_M)} 1 = 1$$

□

For completeness, note that when  $q = 1$ , then  $q_\alpha = 1$  and both  $W_1[\rho_\alpha] = W_1[\rho] = 1$  as one expects.

The rescaling behavior in this property is automatically inherited by the Shannon, Rényi and Tsallis entropies, as pointed out in the next property.

**Property 5. Entropies transformations**

Let  $q, \alpha \in \mathbb{R}$  and  $\rho$  a probability distribution. Then, the Shannon, Rényi and Tsallis entropies of the differential-escort distributions as

$$\frac{S[\rho_\alpha]}{S[\rho]} = \frac{R_q[\rho_\alpha]}{R_{q\alpha}[\rho]} = \frac{T_q[\rho_\alpha]}{T_{q\alpha}[\rho]} = \alpha \tag{16}$$

*Proof.* Taking into account that  $\frac{1-q_\alpha}{1-q} = \alpha$ , the equality for the Rényi and Tsallis entropies trivially follows from property 4.

The Shannon case could be simply understood as the limit case  $q \rightarrow 1$ , however, for the sake of illustration, we give the pretty simple and nice natural proof:

$$S[\rho_\alpha] = \int_{\Lambda_\alpha} \rho_\alpha(y) \log[\rho_\alpha(y)] dy = \int_{\Lambda} \rho(x) \log[\rho(x)^\alpha] dx = \alpha S[\rho].$$

□

Finally, as a direct consequence of the Jensen inequality we can assert that the Rényi entropy of the transformed density  $\rho_\alpha$  is a concave function of  $\alpha$  when  $\lambda > 1$  and convex when  $\lambda < 1$ . Just as property (5) claims, Shannon entropy has a linear behaviour with the deformation parameter  $\alpha$ . This behaviour is given in the following property.

**Property 6.** *The Rényi entropy of the differential-escort distribution fulfills the following identity:*

$$\operatorname{sgn}\left(\frac{\partial^2 R_\lambda[\rho_\alpha]}{\partial \alpha^2}\right) = \operatorname{sgn}(1 - \lambda). \quad (17)$$

So,  $R_\lambda[\rho_\alpha]$  is concave with  $\alpha$  for  $\lambda > 1$  and convex for  $\lambda < 1$ .

*Proof.* One can easily compute

$$\frac{\partial^2 R_\lambda[\rho_\alpha]}{\partial \alpha^2} = \frac{1 - \lambda}{\left(\int_\Lambda \rho^{\lambda_\alpha}\right)^2} \left[ \int_\Lambda \rho^{\lambda_\alpha} \log^2 \rho \int_\Lambda \rho^{\lambda_\alpha} - \left(\int_\Lambda \rho^{\lambda_\alpha} \log \rho\right)^2 \right].$$

On the other hand, due to Jensen's inequality one has

$$\left(\frac{\int_\Lambda \rho^{\lambda_\alpha} \log \rho}{\int_\Lambda \rho^{\lambda_\alpha}}\right)^2 \leq \frac{\int_\Lambda \rho^{\lambda_\alpha} \log^2 \rho}{\int_\Lambda \rho^{\lambda_\alpha}},$$

So, it is straightforward to have that  $\operatorname{sgn}\left(\frac{\partial^2 R_\lambda[\rho_\alpha]}{\partial \alpha^2}\right) = \operatorname{sgn}(1 - \lambda)$ .  $\square$

## 4 The LMC-Rényi Monotonicity

The concept of monotonicity of a complexity measure was recently presented in [20] and proven for the Fisher-Shannon and Crámer-Rao complexity measures. In this section we analyse the behaviour of the LMC-Rényi complexity measure under the differential-escort transformation, and then we show its monotonicity property. Let us first recall that the LMC-Rényi complexity measure is defined [19, 26, 27] as

$$C_{\lambda,\beta}[\rho] = e^{R_\lambda[\rho] - R_\beta[\rho]}, \quad \lambda < \beta. \quad (18)$$

Note that the case ( $\lambda \rightarrow 1, \beta = 2$ ) corresponds to the plain LMC complexity measure [28]

$$C_{1,2}[\rho] = D[\rho]e^{S[\rho]}, \quad (19)$$

which quantifies the combined balance of the average height of  $\rho(x)$  (also called disequilibrium  $D[\rho] = e^{R_2[\rho]}$ ), and its total spreading. This measure has been related with the *degree of multifractality* of the distribution [29] and widely applied in various contexts from electronic systems to seismic events [26, 30, 31]. It satisfies interesting mathematical properties, such as invariance under scaling and translation transformations, invariance under replication and has a lower bound [26] which is achieved by the uniform densities. Obviously, this complexity measure inherits the regularity of the previous section which together with property 5 allows us to write

**Property 7.** *Let  $\lambda < \beta$  and  $\alpha \in \mathbb{R}$ . Then, the LMC-Rényi complexity of the probability distribution  $\rho$  transforms as*

$$C_{\lambda,\beta}[\rho_\alpha] = (C_{\lambda,\beta}[\rho])^\alpha \quad (20)$$

Moreover a straightforward application of the Jensen inequality allows one to find

**Property 8.** *Let  $\lambda < \beta$ . Then, the LMC-Rényi complexity of the probability distribution  $\rho$  is bounded as*

$$C_{\lambda,\beta}[\rho] \geq 1, \quad (21)$$

and the equality trivially holds when  $\rho$  belongs to the class  $\Xi$  of uniform distributions:

$$\Xi = \{\chi^{(a)}(x - x_0) \mid a > 0, x_0 \in \mathbb{R}\}, \quad \chi^{(a)}(x) = \begin{cases} a^{-1}, & x \in [0, a] \\ 0, & \text{otherwise} \end{cases}. \quad (22)$$

So, the LMC-Rényi complexity measure is universally bounded, and the family of minimizing densities is given by the class of uniform densities  $\Xi$ . Actually, this class remains invariant under differential-escort transformations. In fact, restricting us to  $\Xi$ , the transformation  $\mathfrak{E}_\alpha$  just corresponds with a scaling change.

**Property 9. Uniformity transformations**

Let  $\alpha \in \mathbb{R}$ . Then,

$$\rho \in \Xi \iff \mathfrak{E}_\alpha[\rho] \in \Xi, \quad \alpha \neq 0, \quad (23)$$

Particularly, one has that  $\mathfrak{E}_\alpha[\chi^{(a)}] = \chi^{(a^\alpha)}$ .

*Proof.* For any real  $\alpha$ , one has

$$[\chi^{(a)}(x)]^\alpha = a^{-\alpha}, \quad \forall x \in [0, a]$$

and  $dy = a^{\alpha-1}dx$  from Eqs. (6) and (7), respectively. Then, with  $y(0) = 0$  one has that  $y(x)$  obeys the linear relation  $y(x) = a^{\alpha-1}x$ . And by taking into account that  $y([0, a]) = [0, a^\alpha]$  one obtains

$$\mathfrak{E}_\alpha[\chi^{(a)}](y) = [\chi^{(a)}(x(y))]^\alpha = a^{-\alpha}, \quad \forall y \in [0, a^\alpha]$$

or equivalently  $\mathfrak{E}_\alpha[\chi^{(a)}] = \chi^{(a^\alpha)}$ . □

Let us now show that the LMC-Rényi complexity measure is monotone with respect to the class of differential-escort transformations  $\{\mathfrak{E}_\alpha\}_{\alpha \in [0,1]}$  in the Rudnicki et al sense; this means that  $C[\mathfrak{E}_\alpha[\rho]] \leq C[\rho]$  for any density  $\rho$ . We will see that this inequality is a direct consequence of the concavity of

the Rényi entropy 6 with respect to the parameter of the deformation  $\alpha$ .

First we observe that

$$\frac{\partial^2 R_\lambda[\rho_\alpha]}{\partial \lambda \partial \alpha} = \frac{-\alpha}{1-\lambda} \frac{\partial^2 R_\lambda[\rho_\alpha]}{\partial^2 \alpha}, \quad (24)$$

which together with property 6 gives

$$\text{sgn} \left( \frac{\partial^2 R_\lambda[\rho_\alpha]}{\partial \lambda \partial \alpha} \right) = -\text{sgn}(\alpha). \quad (25)$$

Then, if we consider the derivative with respect to  $\alpha$  we have that  $\frac{\partial C_{\lambda,\beta}[\rho_\alpha]}{\partial \alpha} = C_{\lambda,\beta}[\rho_\alpha] \left( \frac{\partial R_\lambda[\rho_\alpha]}{\partial \alpha} - \frac{\partial R_\beta[\rho_\alpha]}{\partial \alpha} \right)$ , and so taking into account that  $\lambda < \beta$  one has

$$\text{sgn} \left( \frac{\partial C_{\lambda,\beta}[\rho_\alpha]}{\partial \alpha} \right) = -\text{sgn} \left( \frac{\partial^2 R_\lambda[\rho_\alpha]}{\partial \lambda \partial \alpha} \right) = \text{sgn}(\alpha) \quad (26)$$

So, from Eq. (26) it trivially follows the searched property:

**Property 10.** *Let  $\lambda < \beta$ . Then, the LMC-Rényi complexity of the probability distribution  $\rho$  fulfills that*

$$C_{\lambda,\beta}[\rho_{\alpha'}] \geq C_{\lambda,\beta}[\rho_\alpha]$$

for any  $\alpha' > \alpha > 0$  or  $\alpha' < \alpha < 0$ . Moreover, if  $\rho \notin \Xi$  the equality only holds for  $\alpha = 1$  and the minimal value is only obtained when  $\alpha = 0$ . In the case that  $\rho \in \Xi$ , then  $C_{\lambda,\beta}[\mathfrak{E}_\alpha[\rho]] = C_{\lambda,\beta}[\rho] = 1$ .

Even more, for  $\alpha = 0$  the minimal possible value of the complexity measure is reached,  $C_{\lambda,\beta}[\mathfrak{E}_0[\rho]] = 1$ . That is due to, for any  $\rho$  one has that  $\mathfrak{E}_0[\rho] = \chi^{(1)}$  as it is claimed in property ??.

The last three properties can be summarized by means of the following theorem:

**Theorem 1.** *Given the family of uniform distributions  $\Xi$ , and the class of transformations  $\mathfrak{E}_\alpha$ , then the triplet  $(C_{\lambda,\beta}, \Xi, \mathfrak{E}_\alpha)$  satisfies the monotonicity property of the LMC-Rényi measure of complexity.*

The comparison of this result with the monotonicity property of the Crámer-Rao and Fisher-Shannon complexity measures obtained by Rudnicki et al. [20] allows us to observe that the class of differential-escort operations play for the LMC-Rényi measure of complexity the same role than the class of convolution-with-the-Gaussian operations in the Crámer-Rao and Fisher-Shannon cases.

## 5 Low and high complexity limits

In this section we conduct a study of the behaviour of the statistical properties of a general density, when deformed in extreme cases  $\alpha \sim 0$  and  $\alpha \rightarrow +\infty$ . To this end, we will first give three statements for the general case that will be useful in the study of the limit cases.

**Proposition 1.** *Let  $\rho(x)$  a bounded density, then the entropic moments  $W_\lambda[\rho]$  satisfies*

$$W_\lambda[\rho] < \infty \iff \lambda > \lambda_c[\rho]$$

with  $\lambda_c[\rho] < 1$ .

For example, for an exponential-like decaying density one has  $\lambda_c[\rho] = 0$ , but for a power-law decaying density as  $\mathcal{O}(x^{-\beta})$  then  $\lambda_c[\rho] = 1/\beta \in (0, 1)$ , or for any N-piecewise density  $\lambda_c[\rho] = -\infty$ . On the other hand, it is easy to see that

$$\lambda_c[\rho_\alpha] = 1 - \frac{1 - \lambda_c[\rho]}{\alpha}. \quad (27)$$

Deserves noting that if we take  $\alpha_c = 1 - \lambda_c[\rho]$  then  $\lambda_c[\rho_{\alpha_c}] = 0$ , what means that  $\rho_{\alpha_c}$  has an infinite support  $W_0[\rho_{\alpha_c}] = W_{\lambda_c}[\rho] = \infty$ , but all entropic moments with positive parameter  $\lambda$  are finite.

On the other hand, is easy to see that the LMC-Rényi complexity measure is not only bounded inferiorly but also superiorly.

**Proposition 2.** *For any density  $\rho \notin \Xi$  and any pair  $\lambda < \beta$  then*

$$1 < C_{\lambda,\beta}[\rho] < C_{\lambda,\infty}[\rho] = \frac{\rho_{max}}{\langle \rho^{\lambda-1} \rangle^{\frac{1}{\lambda-1}}} \quad (28)$$

contrary if  $\rho \in \Xi$  then  $C_{\lambda,\beta}[\rho] = C_{\lambda,\infty}[\rho] = 1$ .

Finally, the third proposition is achieved through the Taylor series of the Rényi entropy  $R_\lambda[\rho]$  on its entropic parameter around  $\lambda = 1$ .

**Proposition 3.** *Given any probability density  $\rho$ , then the associated LMC-Rényi measure can be formally expressed as*

$$C_{\lambda,\beta}[\rho] = e^{\frac{\mathfrak{R}_2[\rho]}{2}(\beta-\lambda)} \prod_{n=2}^{\infty} e^{\frac{\mathfrak{R}_{n+1}[\rho]}{(n+1)!}[(\beta-1)^n - (\lambda-1)^n]},$$

where the quantities  $\mathfrak{K}_n[\rho] = \left. \frac{d^n \log(\rho^{\lambda-1})}{d\lambda^n} \right|_{\lambda=1}$  have the same structure than the cumulants  $k_n = \left. \frac{d^n \log(e^{px})}{dp^n} \right|_{p=0}$ , i.e.,

$$\begin{aligned} \mathfrak{K}_0[\rho] &= 0, \\ \mathfrak{K}_1[\rho] &= -S[\rho] = \langle \log \rho \rangle \\ \mathfrak{K}_2[\rho] &= \langle \log^2 \rho \rangle - \langle \log \rho \rangle^2, \\ \mathfrak{K}_3[\rho] &= \langle \log^3 \rho \rangle - 3\langle \log^2 \rho \rangle \langle \log \rho \rangle + 2\langle \log \rho \rangle^3 \\ &\dots \end{aligned}$$

and provided that the series is convergent. Particularly

$$C_{1,2}[\rho] \equiv C_{LMC}[\rho] = e^{\frac{\mathfrak{K}_2[\rho]}{2}} e^{\frac{\mathfrak{K}_3[\rho]}{3!}} e^{\frac{\mathfrak{K}_4[\rho]}{4!}} \dots$$

It is specially interesting that, for  $\lambda, \beta \sim 1$  we can write

$$C_{\lambda,\beta}[\rho] \simeq e^{\frac{\mathfrak{K}_2[\rho]}{2}(\beta-\lambda)} \quad (29)$$

and when  $\rho \in \Xi$ , then  $C_{\lambda,\beta}[\rho] = e^{\frac{\mathfrak{K}_2[\rho]}{2}(\beta-\lambda)} = 1$ ,  $\forall \lambda < \beta$ .

On the other hand it is straightforward to see that

**Property 11.** Given any probability density  $\rho$  and any  $\alpha \in \mathbb{R}$  then

$$\mathfrak{K}_n[\rho_\alpha] = \alpha^n \mathfrak{K}_n[\rho], \quad (30)$$

and then it follows that  $\frac{\mathfrak{K}_{n+1}[\rho_\alpha]}{\mathfrak{K}_n[\rho_\alpha]} = \alpha \frac{\mathfrak{K}_{n+1}[\rho]}{\mathfrak{K}_n[\rho]}$ .

## Low complexity

Given any probability density  $\rho$ , and choosing a real number  $\alpha \simeq 0$ , then following the Theorem 1 one can always consider that  $\rho_\alpha$  is a low complexity density (in the LMC-sense). First, we note that when  $\alpha \rightarrow 0$ , Eq. (27) diverges, so

**Proposition 4.** Let  $\rho(x)$  a bounded and low complexity density, then the critical entropic parameter  $\lambda_c[\rho] \ll 0$ .

On the other hand, the upper bound of the LMC-Rényi measure of a low complexity density goes to the unity, in such way that Eq (28) is crushed.

$$1 < C_{\lambda,\beta}[\rho_\alpha] < C_{\lambda,\infty}[\rho]^\alpha, \quad \alpha \simeq 0 \quad (31)$$

**Proposition 5.** *For a low complexity density one has that*

$$1 < C_{\lambda,\beta}[\rho] < C_{\lambda,\infty}[\rho], \quad (32)$$

but,  $C_{\lambda,\infty}[\rho] \simeq 1$ .

Finally, taking the Taylor series of  $R_\lambda[\rho_\alpha]$  around  $\alpha = 0$  one obtains  $C_{\lambda,\beta}[\rho_\alpha] \sim e^{\alpha^2 \mathfrak{K}_2[\rho] \frac{(\beta-\lambda)}{2}}$ , but just taking into account property 11, then  $e^{\alpha^2 \mathfrak{K}_2[\rho] \frac{(\beta-\lambda)}{2}} = e^{\mathfrak{K}_2[\rho_\alpha] \frac{(\beta-\lambda)}{2}}$ . That is to say, we can assure that

**Proposition 6.** *If  $\rho$  is a "low complexity density in the LMC-sense", then for any fixed  $\lambda < \beta \ll \infty$*

$$C_{\lambda,\beta}[\rho] \simeq e^{\frac{\mathfrak{K}_2[\rho]}{2}(\beta-\lambda)}. \quad (33)$$

In fact, note that taking into account property 11, the lowest *entropic cumulants*  $\mathfrak{K}_n[\rho]$  domain for the *low complexity* densities. Moreover, in these cases one typically has that  $\mathfrak{K}_{n+1}[\rho] < \mathfrak{K}_n[\rho]$ .

## High complexity

In order to explore the high complexity limit, one can take any probability density  $\rho$ , and a very large  $\alpha \gg 1$ . So, following Theorem 1 one can claim that  $\rho_\alpha$  is a *high complexity* density. First of all, note that the critical entropic parameter  $\lambda_c[\rho]$  of a high complexity density is closed to one (27).

**Proposition 7.** *Let  $\rho(x)$  a bounded and high complexity density, then the critical entropic parameter  $\lambda_c[\rho] \lesssim 1$ .*

On the other hand, the inequality (28) losses the upper bound

**Proposition 8.** *For a high complexity density  $\rho$  one has that*

$$1 < C_{\lambda,\beta}[\rho] < C_{\lambda,\infty}[\rho], \quad (34)$$

but,  $C_{\lambda,\infty}[\rho] \gg 1$ , for any fixed  $\lambda \ll \infty$ .

Finally, it deserves to note that, although Eq. 29 must be valid for values of the parameters  $\lambda$  and  $\beta$  enough close to one, for fixed  $\lambda$  and  $\beta$  is possible to find a density enough complex, in such way that Eq. 29 is not satisfied. In fact  $C_{\lambda,\beta}[\rho_\alpha] = C_{\lambda_\alpha,\beta_\alpha}[\rho]^\alpha \simeq e^{\frac{\mathfrak{K}_2[\rho]}{2}(\beta-\lambda)\alpha^2} = e^{\frac{\mathfrak{K}_2[\rho_\alpha]}{2}(\beta-\lambda)}$ , whenever  $\lambda_\alpha \simeq 1$  and  $\beta_\alpha \simeq 1$ ; that is to say  $\alpha(\lambda - 1) \simeq 0$  and  $\alpha(\beta - 1) \simeq 0$ .

Moreover, taking into account Eq. (11), for a *high complexity* density the highest order entropic cumulants  $\mathfrak{K}_n[\rho]$  will be dominants.

**Proposition 9.** *If  $\rho$  is a high complexity density, then the domain of parameters  $\lambda, \beta$  for what Eq. (29) remain valid is extremely tiny. In fact, the highest order entropic cumulants  $\mathfrak{K}_n[\rho]$  domain the behaviour of the LMC-Rényi complexity measure, in fact, typically  $\mathfrak{K}_{n+1}[\rho] > \mathfrak{K}_n[\rho]$ .*



## Example

In the following we give an example with numerical values. Note that, due to LMC-Rényi is invariant under replication transformation the number  $N$ , of different regions does not play a relevant role in the behaviour of this complexity measure. So, for our purpose it is enough a simple example with  $N = 3$ .

We are going to represent a initial distribution with three steps whose height are  $h_1 = \frac{3}{2}$ ,  $h_2 = 1$ ,  $h_3 = \frac{1}{2}$  and their weights are  $w_1 = w_2 = w_3 = \frac{1}{3}$ . In Figure 1 we show the complexity reduction process through the here studied transformation

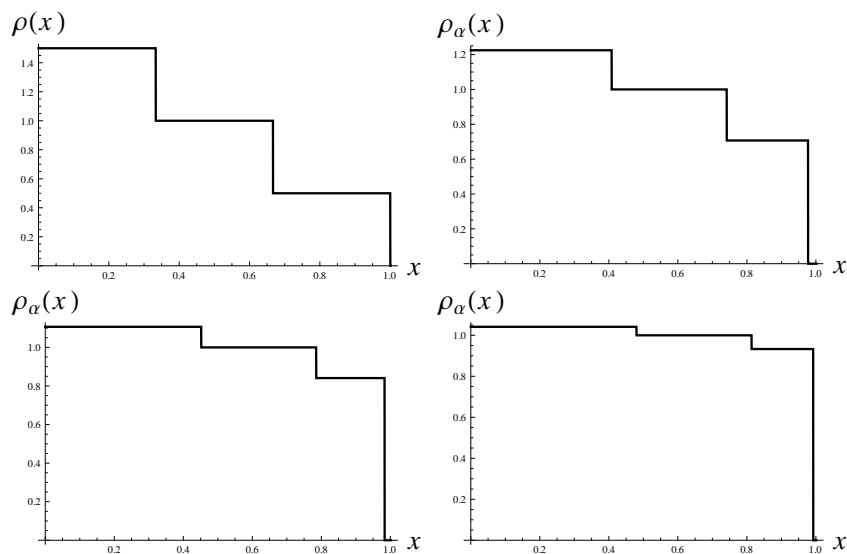


Figure 1: Transformed density  $\rho_\alpha(x)$  for different values of the transformation parameter  $\alpha = 1, \frac{1}{2}, \frac{1}{4}, \frac{1}{10}$ .

It is interesting to give the values of the LMC complexity for this distributions,  $C_{LMC}[\rho_\alpha] \simeq 1.06923, 1.01818, 1.00468, 1.00076$  for  $\alpha = 1, 0.5, 0.25, 0.1$  respectively. In Figure 2 we represent the complexity increasing of this probability density

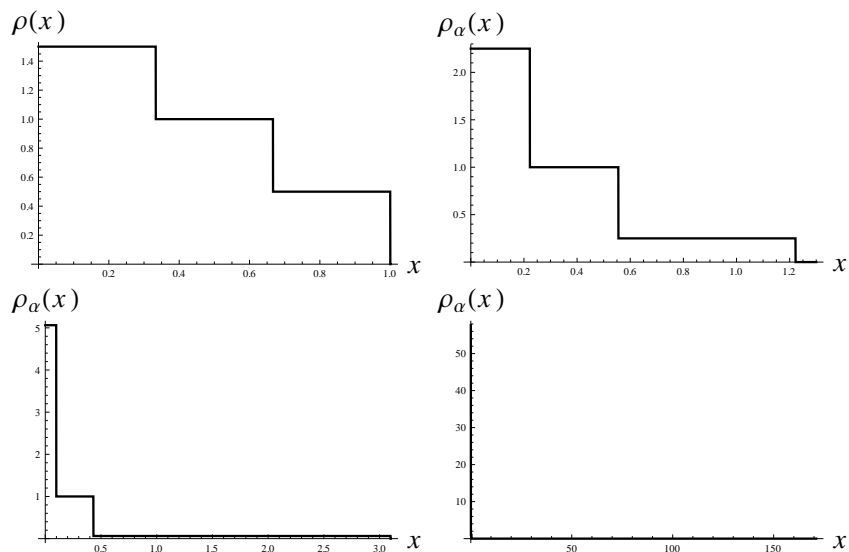


Figure 2: Transformed density  $\rho_\alpha(x)$  for different values of the transformation parameter  $\alpha = 1, 2, 4, 10$ .

Note that, in the case  $\alpha = 10$ , one has that  $(w_1)_\alpha \simeq 0.008$  and  $(h_1)_\alpha \simeq 57$ ,  $(w_2)_\alpha \simeq 0.03$  and  $(h_2)_\alpha = 1$  and finally  $(w_3)_\alpha \simeq 170$  and  $(h_3)_\alpha \simeq 0.001$ . So, in this case the graphic representation is really difficult to be performance. For the sake of illustration, we give the case  $\alpha = 100$ , for which  $(w_1)_\alpha \simeq 10^{-18}$  and  $(h_1)_\alpha \simeq 4 \times 10^{17}$ ,  $(w_2)_\alpha \simeq 0.03$  and  $(h_2)_\alpha = 1$  and finally  $(w_3)_\alpha \simeq 2 \times 10^{29}$  and  $(h_3)_\alpha \simeq 7 \times 10^{-31}$ , what seems to be near to impossible to be graphically resented with accuracy (even using a logarithmic scale in both axes) while still being a 3-piecewise density. The values of the LMC complexity for these densities are  $C_{LMC}[\rho_\alpha] \simeq 1.06923, 1.25988, 2.02809, 12.1843, 3 \times 10^{13}$  for  $\alpha = 1, 2, 4, 10, 100$  respectively.

## 6 q-exponential and power-law decaying densities

The exponential and q-exponential distributions are fundamental tools in the extensive and non-extensive formalisms [22]. They can be obtained by maximizing the Rényi and Tsallis entropies with a suitable constraint[16], or by maximizing Shannon entropy with some tail constraints [23]. In this section we will study the q-exponential distribution in the framework of the differential-escort transformations which will able to naturally relate it to the exponential one.

The exponential function  $\mathcal{E}(x) = e^{-x}$ , with  $x \in [0, \infty)$ , is recovered taking the limit  $q \rightarrow 1$  in the family of q-exponential functions defined by

$$e_q(x) = (1 + (1 - q)x)_+^{\frac{1}{1-q}} \quad (35)$$

where  $(t)_+ = \max\{t, 0\}$ . Tsallis introduced [16] the q-exponential probability densities which are proportional to  $e_q(-x)$ . For convenience, we denote the q-exponential densities as

$$\mathcal{E}_q(y) \equiv e_q\left(-\frac{y}{2-q}\right). \quad (36)$$

Note that when  $q \in (1, 2)$  the support is non compact and the tail of the probability density decays as a heavy-tailed distribution; in contrast when  $q < 1$ , the support is compact.

It is worth to realize that the standard escort transformation of a q-exponential density is another q-exponential; indeed,

$$E_\alpha[\mathcal{E}_q] = \mathcal{E}_{q'}, \quad q' = 1 + \frac{q-1}{\alpha} \quad (37)$$

Note that, if  $q = 1$  then  $q' = 1$ ; that is to say, the escort transformation of an exponential distribution is another exponential distribution. On the other hand, if  $q > 1$  the support of  $\mathcal{E}_q$  is not compact and so necessarily  $\alpha > q - 1 > 0$  for the sake of satisfying the convergence condition given in (1); and in consequence, when  $q \in (1, 2)$  necessarily  $q' \in (1, 2)$ . Finally, when  $q < 1$  one has that  $q' < 1$  for any  $\alpha > 0$ . In other words, the escort transformation  $E_\alpha$  keep unchanged the three regions of the parameter  $q$  ( $q < 1, q = 1, q > 1$ ); this behaviour is expected since the standard escort transformation keep the support invariant.

This behaviour is totally different for the differential-escort transformation, which indeed changes the length of the support. In fact, it transforms not only a q-exponential distribution in another one, but also: given any initial value of the parameter  $q < 2$ , any other parameter  $q' < 2$  can be obtained through the use of  $\mathfrak{E}_\alpha$  with  $\alpha \neq 1$ , as we shall see below.

From definition 1, given any  $\alpha$  one has that

$$\mathfrak{E}_\alpha[\mathcal{E}](y) = e^{-\alpha x(y)} \quad (38)$$

with

$$y(x) = \int_0^x e^{(\alpha-1)t} dt = \frac{1}{\alpha-1} (e^{(\alpha-1)x} - 1), \quad \alpha \neq 1 \quad (39)$$

and so one easily obtains

$$x(y) = \frac{1}{\alpha - 1} \log(1 + (\alpha - 1)y) \quad (40)$$

So, inserting (40) in (38) we have that

$$\mathfrak{E}_\alpha[\mathcal{E}](y) = (1 + (\alpha - 1)y)^{\frac{\alpha}{1-\alpha}}, \quad (41)$$

where, from Eq. (39),  $y \in [0, \infty]$  for  $\alpha > 1$  and  $y \in [0, \frac{1}{1-\alpha}]$  when  $\alpha < 1$ . In fact, we can rewrite Eq. (41) as

$$\mathfrak{E}_\alpha[\mathcal{E}](y) = e^{\frac{2\alpha-1}{\alpha}(-\alpha y)}. \quad (42)$$

Or equivalently, choosing  $\alpha = \frac{1}{2-q}$  and using the notation introduced in Eq. (36), one can write

$$\mathfrak{E}_{\frac{1}{2-q}}[\mathcal{E}] = \mathcal{E}_q. \quad (43)$$

On the other hand, taking into account that  $\mathfrak{E}_1[\rho] = \rho$  and considering the composition property 2 and Eq. (43) one obtains the identities

$$\mathfrak{E}_{2-q}[\mathcal{E}_q] = \mathfrak{E}_{2-q}[\mathfrak{E}_{\frac{1}{2-q}}[\mathcal{E}]] = \mathfrak{E}_{\frac{2-q}{2-q}}[\mathcal{E}] = \mathcal{E}, \quad \forall q < 2 \quad (44)$$

From which, taking any couple  $q, \bar{q} < 2$  one can write the following relation between q-exponential densities

$$\mathfrak{E}_{2-q}[\mathcal{E}_q] = \mathfrak{E}_{2-\bar{q}}[\mathcal{E}_{\bar{q}}] \quad (45)$$

or equivalently, using again the composition property,

$$\mathfrak{E}_{\frac{2-q}{2-\bar{q}}}[\mathcal{E}_q] = \mathcal{E}_{\bar{q}} \quad (46)$$

or as well  $\mathfrak{E}_\alpha[\mathcal{E}_q] = \mathcal{E}_{\bar{q}}$  with

$$\bar{q} = 2 + \frac{q-2}{\alpha} \quad (47)$$

Thus, as we have previously anticipated, starting with any  $q < 2$  we can obtain any other value  $\bar{q} < 2$ . In particular, when  $\bar{q} > 1$  it occurs that  $\alpha > 2 - q$ , when  $\bar{q} = 1$  one has  $\alpha = 2 - q$ , and when  $\bar{q} < 1$  it happens that  $\alpha < 2 - q$ . Note that the value  $\alpha = 2 - q$  plays a critical role. Finally, it is worth mentioning that, when  $\alpha > 0$  then  $\bar{q} < 2$ , but taking  $\alpha < 0$  one obtains  $\bar{q} > 2$  which normally is not considered, however note that these densities are correctly defined and they satisfy the normalization condition  $\int_{\Lambda_\alpha} \rho_\alpha(y) = 1$ .

These results are a little bit extended in the next lemma:

**Lemma 1.** *Let  $\rho(x) > 0, \forall x \in [0, \infty)$ , be a probability density, such that the tail of  $\rho(x)$  decreases as  $\mathcal{O}(x^{-\beta})$ ,  $\beta > 1$ . Then, for  $\alpha > \alpha_c = \frac{\beta-1}{\beta}$ , the tail of the transformed distribution  $\rho_\alpha(y)$  decreases as  $\mathcal{O}\left(y^{\frac{-\beta\alpha}{1-\beta(1-\alpha)}}\right)$ . On the other hand, for  $\alpha < \alpha_c$ , the distribution  $\rho_\alpha$  has a compact support. Finally, when  $\alpha = \alpha_c$  the support is non-compact and there is an exponential decay.*

*Proof.* Let  $\alpha \in \mathbb{R}$ .

Given  $x \gg 1$ , the original density fulfilled  $\rho(x) \sim x^{-\beta}$ . On the other hand the variable change is defined as  $y(x) = \int_0^x [\rho(t)]^{1-\alpha} dt$ . Then, the length of the support of  $\rho_\alpha$  is given by  $W_0[\rho_\alpha] = W_{1-\alpha}[\rho] = \int_0^\infty \rho(x)^{1-\alpha} dx \sim \int_{a>0}^\infty x^{-\beta(1-\alpha)}$ . So, it is clear that the support of  $\rho_\alpha$  is compact iff  $\alpha < \frac{\beta-1}{\beta}$ , and in the case  $\alpha \geq \frac{\beta-1}{\beta}$  we have that  $\lim_{x \rightarrow \infty} y(x) \rightarrow \infty$ .

In the case  $\alpha \geq \frac{\beta-1}{\beta}$ , one can suppose  $x \gg 1$ , and so  $\rho_\alpha(y) \propto [x(y)]^{-\beta\alpha}$ , and in the other hand  $\frac{dy}{dx} = \rho(x)^{1-\alpha} \propto x^{-\beta(1-\alpha)}$ .

Note that when  $\alpha = \alpha_c = \frac{\beta-1}{\beta}$ , then  $-\beta(1-\alpha) = -1$ , and so  $y(x) \propto \ln x$ , or equivalently  $x(y) \propto e^y$ . In this case we have that  $\rho_\alpha(y) \propto [x(y)]^{-\beta\alpha} \propto e^{-(\beta-1)y}$ .

Finally, when  $\alpha > \frac{\beta-1}{\beta}$ , so  $y(x) \propto x^{1-\beta(1-\alpha)}$ ; i.e, when  $x, y \gg 1$  we have that  $x(y) \propto y^{\frac{1}{1-\beta(1-\alpha)}}$ . Thus,  $\rho_\alpha(y) \propto y^{\frac{-\beta\alpha}{1-\beta(1-\alpha)}}$ . □

It is interesting to note that under the conditions of Lemma 1, and in the high complexity limit, all the expected values become to be infinite, as well as the respective entropic moments  $W_\lambda$  when  $\lambda < 1$ . This is in concordance with the proposition 7, which states that, the entropic moments of the density are not well defined in the high complexity limit.

It is known that any distribution is characterized by its standard moments, provided that they exist. However, power-law-decaying probability densities does not fully satisfy this condition. In order to tackle this problem, Tsallis et al. [32] purposed to use escort mean values. This make sense, taking into account that the escort density has more well defined moments than the original ones by choosing adequately the escort parameter. However, note that all escort transformation of a heavy tailed density remains being a heavy tailed, that is to say, a dense set of moments (with real parameter) remains always infinite. Contrary, as stated by Lemma 1, through the differential-escort density, we can always find a probability density which all its real moments correctly defined, at least for power-law-decaying probability densities. For these reasons, the characterization via *differential escort* densities seems to be more accurate than via escort ones.

## 7 Conclusions

In this paper we have presented the concept of differential-escort transformation of a univariate probability density. Its basic mathematical properties as composition and strong probability invariance have been studied. Then, we have shown the regular behaviour of the Shannon, Rényi and Tsallis entropies for the differential-escort distributions. Moreover, the convex behaviour of the Rényi entropy with respect to the differential-escort operation has been the keystone in the proof of the monotonicity property of the LMC-Rényi complexity measure. Note that the differential-escort operation allows to define equivalence classes of probability densities where exists a total order with respect to their LMC-Rényi complexity. Later we have analysed the statistical properties of a general probability density when it is deformed to both extreme complexity cases, the low and high complexity limits. Finally, we have studied the behaviour of the exponential and q-exponential densities, showing not only the stability of the q-exponential family, but also the existence of a critical value of the deformation parameter for what the behaviour of the tail, if any, dramatically changes to an exponential one.

Interestingly, the action of this operation over a probability density allows for a clear interpretation of the probability conservation. Indeed, the conservation of the probability in any region of the transformed-space is clear by construction, what has a clear mass conservation interpretation.

On the other hand, the simplicity of the differential-escort transformations together with the general character of the presented results seem to indicate that this way of thinking would deserve to be explored from a more general point of view. Let us advance for example that the use of a differential-escort-based methodology has allowed for a huge generalization of the Stam inequality [33].

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## Chapter 7

# Generalized Stam inequality and triparametric Fisher-Rényi complexity

In this chapter we introduce a triparametric complexity measure of Fisher–Rényi type by means of a generalization of the biparametric Stam inequality for univariate probability densities [119]. To do this we use two complementary approaches. First, we obtain the triparametric Stam inequality by means of the Gagliardo-Nirenberg inequality, finding a differential equation for the minimizing family of functions but we cannot not give any information about the minimal bound beyond its mere existence; the exact solution can be derived following the variational approach Agueh [269, 270] only for some particular cases of the involved parameters. On the other hand, the regular behaviour of the biparametric Fisher information with respect to differential-escort transformations allows us not only to find the exact bound and the explicit expression for the family of minimizing densities, but also allows to extend the validity domain of the inequality beyond that Gagliardo-Nirenberg approach can do. Finally, the triparametric Fisher-Rényi complexity measure is given and applied to the harmonic and hydrogenic systems.

Summarizing, we have carried out the following tasks:

- We define the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity  $C_{p,\beta,\lambda}[\rho]$  of the probability density  $\rho$ .
- We show that the biparametric Fisher information (1.19) has the following regular behavior with respect to the differential-escort transformations  $\mathfrak{E}_\alpha$  for a one-dimensional probability density  $\rho$ .

$$F_{p,\beta}[\mathfrak{E}_\alpha[\rho]] = |\alpha|^p F_{p,\alpha\beta}[\rho], \quad p > 1, \beta \in \mathbb{R}_+^*. \quad (7.1)$$

- We compute an explicit expression for the family of minimizing densities; namely the generalized  $(p, \beta, \lambda)$ -Gaussian densities,  $g_{p,\beta,\lambda}$ , which are given for  $p > 1$  and  $(\beta, \lambda) \in \mathbb{R}_+^{*2}$  as

$$g_{p,\beta,\lambda}(x) \propto \begin{cases} \left[ 1 - \mathfrak{B}^{-1}\left(\frac{1}{p^*}, q_{p,\beta,\lambda}; \frac{p^*|x|}{|1-\lambda|p^*}\right) \right]^{\frac{1}{|1-\lambda|}} \mathbf{1}_{[0;B(\frac{1}{p^*}, q_{p,\beta,\lambda})]} \left( \frac{p^*|x|}{|1-\lambda|p^*} \right), & \text{if } \lambda \neq 1, \\ \exp\left(-\frac{\mathfrak{G}^{-1}\left(\frac{1}{p^*}; \left(\frac{\beta-1}{\beta}\right)^{\frac{1}{p^*}} p^*|x|\right)}{\beta-1}\right) \mathbf{1}_{\left[0; \frac{\Gamma(1/p^*)}{\Gamma(0;1)^{(\beta)}}\right]}(p^*|x|), & \text{if } \begin{matrix} \lambda = 1, \\ \beta \neq 1, \end{matrix} \\ g_{p,\lambda}(x), & \text{if } \beta = \lambda, \end{cases}$$

with<sup>1</sup>

$$q_{p,\beta,\lambda} = \frac{\beta-1}{|1-\lambda|} + \frac{\mathbf{1}_{\mathbb{R}_+}(1-\lambda)}{p}. \quad (7.2)$$

The symbols  $\mathfrak{B}^{-1}(x)$ ,  $\mathfrak{G}^{-1}(x)$  and  $\mathbf{1}_{[a;b]}(x)$  denote the inverse beta function, the inverse gamma function and the indicator function, respectively [59].

- We show that the  $(p, \beta, \lambda)$ -Fisher-Rényi complexity has the following non-trivial lower bound

$$\forall p > 1, \quad (\beta, \lambda) \in \tilde{\mathcal{D}}_p = \{(\beta, \lambda) \in \mathbb{R}_+^{*2} : \lambda > 1 - \beta p^*\}, \quad C_{p,\beta,\lambda}[\rho] \geq K_{p,\beta,\lambda} \quad (7.3)$$

The minimizers are explicitly given by the the  $(p, \beta, \lambda)$ -Gaussian as

$$\arg \min_{\rho} C_{p,\beta,\lambda}[\rho] = g_{p,\beta,\lambda} \quad (7.4)$$

and the lower bound is

$$K_{p,\beta,\lambda} = \begin{cases} \left( \frac{2}{p^* \zeta_{p,\beta,\lambda}} \left( \frac{p^* \zeta_{p,\beta,\lambda}}{|1-\lambda|} \right)^{\frac{1}{p^*}} \left( \frac{p^* \zeta_{p,\beta,\lambda}}{p^* \zeta_{p,\beta,\lambda} - |1-\lambda|} \right)^{\frac{\zeta_{p,\beta,\lambda}}{|1-\lambda|} + \frac{1}{p}} B\left(\frac{1}{p^*}, \frac{\zeta_{p,\beta,\lambda}}{|1-\lambda|} + \frac{1}{p}\right) \right)^2 & \text{if } \lambda \neq 1 \\ \left( \frac{2 e^{\frac{1}{p^*}} \Gamma\left(\frac{1}{p^*}\right)}{\beta p^* \frac{1}{p}} \right)^2 & \text{if } \lambda = 1 \end{cases} \quad (7.5)$$

with

$$\zeta_{p,\beta,\lambda} = \beta + \frac{(\lambda-1)_+}{p^*} \quad (7.6)$$

- We numerically study the tri-parametric Fisher-Rényi complexity measure of the radial density of the harmonic and hydrogenic systems for the lowest energy states.

<sup>1</sup>The choice of scaling allows to recover precisely def. 4.7 with the same scaling when  $\beta = \lambda$ .

These results have been published in the article [69] with coordinates: Zozor, S., **Puertas-Centeno, D.** and Dehesa, J. S. *On Generalized Stam Inequalities and Fisher-Rényi Complexity Measures*. Entropy, 19:493, 2017, which is attached below.

# On Generalized Stam Inequalities and Fisher–Rényi Complexity Measures

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Information-theoretic inequalities play a fundamental role in numerous scientific and technological areas (e.g., estimation and communication theories, signal and information processing, quantum physics, . . .) as they generally express the impossibility to have a complete description of a system via a finite number of information measures. In particular, they gave rise to the design of various quantifiers (statistical complexity measures) of the internal complexity of a (quantum) system. In this paper, we introduce a three-parametric Fisher–Rényi complexity, named  $(p, \beta, \lambda)$ -Fisher–Rényi complexity, based on both a two-parametric extension of the Fisher information and the Rényi entropies of a probability density function  $\rho$  characteristic of the system. This complexity measure quantifies the combined balance of the spreading and the gradient contents of  $\rho$ , and has the three main properties of a statistical complexity: the invariance under translation and scaling transformations, and a universal bounding from below. The latter is proved by generalizing the Stam inequality, which lowerbounds the product of the Shannon entropy power and the Fisher information of a probability density function. An extension of this inequality was already proposed by Bercher and Lutwak, a particular case of the general one, where the three parameters are linked, allowing to

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determine the sharp lower bound and the associated probability density with minimal complexity. Using the notion of differential-escort deformation, we are able to determine the sharp bound of the complexity measure even when the three parameters are decoupled (in a certain range). We determine as well the distribution that saturates the inequality: the  $(p, \beta, \lambda)$ -Gaussian distribution, which involves an inverse incomplete beta function. Finally, the complexity measure is calculated for various quantum-mechanical states of the harmonic and hydrogenic systems, which are the two main prototypes of physical systems subject to a central potential.

*Keywords:*  $(p, \beta, \lambda)$ -Fisher–Rényi complexity; extended sharp Stam inequality;  $(p, \beta, \lambda)$ -Gaussian distributions; application to  $d$ -dimensional central potential quantum systems

## 1 Introduction

The definition of complexity measures to quantify the internal disorder of physical systems is an important and challenging task in science, basically because of the many facets of the notion of disorder [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. It seems clear that a unique measure is unable to capture the essence of such a vague notion. In the scalar continuous-state context we consider in this paper, many complexity measures based on the probability distribution describing a system have been proposed in the literature, attempting to capture simultaneously the spreading (global) and the oscillatory (local) behaviors of such a distribution [13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 10, 12, 27, 28, 29]. They mostly depend on entropy-like quantities such as the Shannon entropy [30], the Fisher information [31] and their generalizations. The measures of complexity of a probability density  $\rho$  proposed up until now, say  $C[\rho]$ , making use of two information-theoretic properties, share several properties (see e.g., [32]), such as e.g., the invariance by translation or by a scaling factor (i.e., for any  $x_0 \in \mathbb{R}$  and  $\sigma > 0$ , for  $\tilde{\rho}(x) = \frac{1}{\sigma}\rho\left(\frac{x-x_0}{\sigma}\right)$ , they satisfy  $C[\tilde{\rho}] = C[\rho]$ ). For instance, the disorder may be invariant from a move of a (referential independent) center of mass. Moreover, all the proposed measures are also lowerbounded, which means that there exists in a certain sense a distribution of minimal complexity, which is the probability density that reaches the lower bound.

In this paper, we generalize the complexity measures of global-local character published in the literature (see e.g., [23, 10, 24, 26, 12, 27, 29]) to grasp both the spreading and the fluctuations of a probability density  $\rho$  by the introduction of a three-parametric Fisher–Rényi complexity, which involves the Rényi entropy [33] and generalized Fisher information [34, 36, 35]. The products of these two generalized information-theoretic tools, which are

translation and scaling invariant as well as lowerbounded, can be used as generalized complexity measures of  $\rho$ .

Historically, the first inequality involving the Shannon entropy and the Fisher information was proved by Stam [37] under the form

$$F[\rho]N[\rho] \geq 2\pi e, \tag{1}$$

where  $F$  and  $N$  are, respectively, the (nonparametric) Fisher information of  $\rho$ ,

$$F[\rho] = \int_{\mathbb{R}} \left( \frac{d}{dx} \log[\rho(x)] \right)^2 \rho(x) dx \tag{2}$$

and the Shannon entropy power of  $\rho$ , i.e., an exponential of the Shannon entropy  $H$ ,

$$N[\rho] = \exp(2H[\rho]) \quad \text{where} \quad H[\rho] = - \int_{\mathbb{R}} \rho(x) \log[\rho(x)] dx. \tag{3}$$

In fact, the Fisher information concerns a density parametrized by a parameter  $\theta$  and the derivative is vs  $\theta$ . When this parameter is a position parameter, this leads to the nonparametric Fisher information. Concerning the entropy power, more rigorously, a factor  $\frac{1}{2\pi e}$  affects  $N$  and the bound in the Stam inequality is then unity. This factor does not change anything for our purpose, hence, for sake of simplicity, we omit it. The lower bound in Inequality 1 is achieved for the Gaussian distribution  $\rho(x) \propto \exp(-\frac{1}{2}x^2)$  up to a translation and a scaling factor (where  $\propto$  means “proportional to”). In other words, the so-called *Fisher–Shannon complexity*  $C[\rho] = F[\rho]N[\rho]$ , which is translation and scale invariant, is always higher than  $2\pi e$  (and thus cannot be zero) and the distribution of lowest complexity is the Gaussian, exhibiting (also) through this measure its fundamental aspect. The proof of this inequality lies in the entropy power inequality and on the de Bruijn identity, two information theoretic inequalities, both being reached in the Gaussian context [37, 38]. Although introduced respectively in the estimation context through the Cramér–Rao bound [39, 40, 31] and in communication theory through the coding theorem of Shannon [30, 38], these quantities found applications in physics as previously mentioned (and also in the earlier papers [41, 42] and that of Stam). In particular, the analysis of a signal with these measures was proposed by Vignat and Bercher [43] and the Fisher–Shannon complexity  $C[\rho] = F[\rho]N[\rho]$  is widely applied in atomic physics or quantum mechanics for instance [26, 25, 44, 45, 46, 47].

Recently, the Stam inequality was extended by substituting the Shannon entropy by the Rényi entropies (a family of entropies characterizing by

a parameter playing a role of focus [33]), and the Fisher information by a generalized two-parametric family of the Fisher information introduced by [34, 35, 36]. As we will see later on, this extended inequality involves, however, two free parameters because one of the two Fisher parameters is linked to the Rényi one. This constraint is imposed so as to determine the sharp bound of the inequality and the minimizers in the framework of the (stretched) Tsallis distributions [48, 49]. Thus, this extended inequality allows to define again a complexity measure, based on this generalized Fisher information and the Rényi entropy power [27].

In this paper, we study the full three-parametric Fisher–Rényi complexity, disconnecting the two parameters tuning the extended Fisher information and the parameter tuning the Rényi entropy. Like Bercher, we use an approach based on the Gagliardo–Nirenberg inequality. This inequality allows for proving the existence of a lower bound of the complexity when the parameters are decoupled, in a certain range. The minimizers are thus implicitly known as a solution of a nonlinear equation (or through a complicated series of integrations and inversion of nonlinear functions). Moreover, the sharp bound of the associated extended Stam inequality is explicitly known, once the minimizers have been determined. We propose here an indirect approach allowing (i) to extend a step further the domain where the Stam inequality holds (or where the complexity is non trivially lower-bounded); (ii) to determine explicitly the minimizers; and (iii) to find the sharp bound, regardless of the knowledge of the minimizers.

The structure of the paper is the following. In Section 2, we introduce both the  $\lambda$ -dependent Rényi entropy power and the  $(p, \beta)$ -Fisher information, so generalizing the usual (i.e., translationally invariant) Fisher information. Then, we propose a complexity measure based on these two information quantities, the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity, and we study its fundamental properties regarding the invariance under translation and scaling transformations and, above all, the universal bounding from below. In particular, we come back briefly to the results of Lutwak [34] or of Bercher [35] concerning the sharpness of the bound and the minimizers, derived only when the three parameters belong to a two-dimensional manifold, finding that our results remain indeed valid in a domain slightly wider than theirs. In Section 3, the core of the paper, we come back to the lower bound (or to the extended Stam inequality) dealing with a wide three-dimensional domain. In this extended domain, which includes that of the previous section, we are able to derive explicitly the minimizers and the sharp lower bound, regardless the knowledge of the minimizers. In order to do this, we introduce a special nonlinear stretching of the state, leading to



the so-called differential-escort distribution [50]. This geometrical deformation allows us to start from the Bercher–Lutwak inequality and to introduce a supplementary degree of freedom so as to decouple the parameters (in a certain range). This approach is the key point for the determination of the extended domain where the complexity is bounded from below (the generalized Stam inequality). Moreover, we provide an explicit expression for the densities which minimize this complexity, expression involving the inverse incomplete beta function. In Section 4, we apply the previous results to some relevant multidimensional physical systems subject to a central potential, whose quantum-mechanically allowed stationary states are described by wave functions that factorize into a potential-dependent radial part and a common spherical part. Focusing on the radial part, we calculate the three-parametric complexity of the two main prototypes of  $d$ -dimensional physical systems, the harmonic (i.e., oscillator-like) and hydrogenic systems, for various quantum-mechanical states and dimensionalities. Finally, three appendices containing details of the proofs of various propositions of the paper are reported.

## 2 $(p, \beta, \lambda)$ -Fisher–Rényi Complexity and the Extended Stam Inequality

In this section, we firstly review the extension of the Stam inequality based on the efforts of Lutwak et al. and Bercher [34, 36, 35], or more generally, based on that of Agueh [51, 52]. To this aim, we introduce a three-parametric Fisher–Rényi complexity, showing its scaling and translation invariance and non-trivial bounding from below. We then come back to the results of Lutwak or Bercher concerning the determination of the sharp bound and the minimizers of its associated complexity, where a constraint on the parameters was imposed. Indeed, the constraint they imposed can be slightly relaxed, as we will see in this section.

### 2.1 Rényi Entropy, Extended Fisher Information and Rényi–Fisher Complexity

Let us begin with the definitions of the following information-theoretic quantities of the probability density  $\rho$ : the Rényi entropy power  $N_\lambda[\rho]$ , the  $(p, \beta)$ -Fisher information  $F_{p,\beta}[\rho]$ , and the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity  $C_{p,\beta,\lambda}[\rho]$ .

**Definition 1 (Rényi entropy power [33])** *Let  $\lambda \in \mathbb{R}_+^*$ . Provided that the integral exists, the Rényi entropy power of index  $\lambda$  of a probability density function  $\rho$  is given by*

$$N_\lambda[\rho] = \exp(2H_\lambda[\rho]) \quad \text{where} \quad H_\lambda[\rho] = \frac{1}{1-\lambda} \log \int_{\mathbb{R}} [\rho(x)]^\lambda dx, \quad (4)$$

where the limiting case  $\lambda \rightarrow 1$  gives the Shannon entropy power  $N[\rho] = N_1[\rho] \equiv \lim_{\lambda \rightarrow 1} N_\lambda[\rho]$ .

The entropy  $H_\lambda$  was introduced by Rényi in [33] as a generalization of the Shannon entropy. In this expression, through the exponent  $\lambda$  applied to the distribution, more weight is given to the tail ( $\lambda < 1$ ) or to the head ( $\lambda > 1$ ) of the distribution [34, 53, 54, 55]. This measure found many applications in numerous fields such as e.g., signal processing [56, 57, 58, 59, 60, 61, 62], information theory to reformulate the entropy power inequality [63], statistical inference [64], multifractal analysis [65, 66], chaotic systems [67], or in physics as mentioned in the introduction (see ref. above). For instance, the Rényi entropies were used to reformulate the Heisenberg uncertainty principle (see [68, 69, 70, 71, 72] or [73, 74] where this formulation also appears and is applied in quantum physics).

Whereas the power applied to the probability density  $\rho$  in the Rényi entropy aims at making a focus on heads or tails of the distribution, one may wish to act similarly dealing with the Fisher information. In this case, since both the density and its derivative are involved, one may wish to stress either some parts of the distribution, or some of its variations (small or large fluctuations). Thus, two different power parameters for  $\rho$  and its derivative, respectively, can be considered leading with our notations to the following definition of the bi-parametric Fisher information.

**Definition 2 ( $(p, \beta)$ -Fisher information [34, 36, 35])** *For any  $p \in (1, \infty)$  and any  $\beta \in \mathbb{R}_+^*$ , the  $(p, \beta)$ -Fisher information of a continuously differentiable density  $\rho$  is defined by*

$$F_{p,\beta}[\rho] = \left( \int_{\mathbb{R}} \left| [\rho(x)]^{\beta-1} \frac{d}{dx} \log[\rho(x)] \right|^p \rho(x) dx \right)^{\frac{2}{p\beta}}, \quad (5)$$

provided that this integral exists. When  $\rho$  is strictly positive on a bounded support, the integration is to be understood over this support, but it must be differentiable on the closure of this support.

It is straightforward to see that  $F_{2,1}$  is the usual Fisher information. When it exists,  $\lim_{p \rightarrow +\infty} [F_{p,\beta}]^{\frac{\beta}{2}}$  is the essential supremum of  $|\rho^{\beta-1} \frac{d}{dx} \log[\rho]|$ . Conversely,  $\frac{1}{\beta} [F_{1,\beta}]^{\frac{\beta}{2}}$  is the total variation of  $\rho^\beta$ . For  $p = 2$ , this extended Fisher information is closely related to the  $\alpha$ -Fisher information introduced by Hammad in 1978 when dealing with a position parameter [75]. Note also that a variety of generalized Fisher information was applied especially in non-extensive physics [76, 77, 78, 79].

From the Rényi entropy power and the  $(p, \beta)$ -Fisher information, we define a  $(p, \beta, \lambda)$ -Fisher–Rényi complexity by the product of these quantities, up to a given power.

**Definition 3** ( $(p, \beta, \lambda)$ -Fisher–Rényi complexity) *We define the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity of a probability density  $\rho$  by*

$$C_{p,\beta,\lambda}[\rho] = \left( F_{p,\beta}[\rho] N_\lambda[\rho] \right)^\beta, \quad (6)$$

*provided that the involved quantities exist.*

We choose to elevate the product of the entropy power and Fisher information to the power  $\beta > 0$  for simplification reasons. Indeed, it does not change the spirit of this measure of complexity, whereas it allows to express symmetry properties in a more elegant manner, as we will see later on.

This quantity has the minimal properties expected for a complexity measure (see e.g., [32]), as stated in the next subsection.

## 2.2 Shift and Scale Invariance, Bounding from below and Minimizing Distributions

The first property of the proposed complexity  $C_{p,\beta,\lambda}[\rho]$  is the invariance under the basic translation and scaling transformations.

**Proposition 1** *The  $(p, \beta, \lambda)$ -Fisher–Rényi complexity of the probability density  $\rho$  is invariant under any translation  $x_0 \in \mathbb{R}$  and scaling factor  $\sigma > 0$  applied to  $\rho$ ; i.e., for  $\tilde{\rho}(x) = \frac{1}{\sigma} \rho\left(\frac{x-x_0}{\sigma}\right)$ ,  $C_{p,\beta,\lambda}[\tilde{\rho}] = C_{p,\beta,\lambda}[\rho]$ .*

**proof 1** *This is a direct consequence of a change of variables in the integrals, showing that  $N_\lambda[\tilde{\rho}] = \sigma^2 N_\lambda[\rho]$  (justifying the term of entropy power) for any  $\lambda$ , and that  $F_{p,\beta}[\tilde{\rho}] = \sigma^{-2} F_{p,\beta}[\rho]$ , whatever  $(p, \beta)$ .*

From now, due to these properties, all the definitions related to probability density functions will be given up to a translation and scaling factor.

In other words, when evoking a density  $\rho$ , except when specified, we will deal with the family  $\frac{1}{\sigma} \rho\left(\frac{x-x_0}{\sigma}\right)$  for any  $x_0 \in \mathbb{R}$  and  $\sigma > 0$ .

More important, the complexity has a universal, non-trivial bounding from below so that the distribution corresponding to this minimal complexity can thus be viewed as the less complex one.

**Proposition 2 (Extended Stam inequality)** *For any  $p > 1$ ,*

$$(\beta, \lambda) \in \mathcal{D}_p = \left\{ (\beta, \lambda) \in \mathbb{R}_+^{*2} : \beta \in \left( \frac{1}{p^*}; \frac{1}{p^*} + \min(1, \lambda) \right] \right\}, \quad (7)$$

with  $p^* = \frac{p}{p-1}$  the Holder conjugate of  $p$ , there exists a universal optimal positive constant  $K_{p,\beta,\lambda}$ , that bounds from below the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity of any density  $\rho$ , i.e.,

$$\forall \rho, \quad C_{p,\beta,\lambda}[\rho] \geq K_{p,\beta,\lambda}. \quad (8)$$

The optimal bound is achieved when, up to a shift and a scaling factor,

$$\rho_{p,\beta,\lambda} = u^\vartheta \quad \text{with} \quad \vartheta = \frac{p^*}{\beta p^* - 1}, \quad (9)$$

and where  $u$  is a solution of the differential equation

$$-\frac{d}{dx} \left( \left| \frac{d}{dx} u \right|^{p-2} \frac{d}{dx} u \right) + \frac{\gamma}{\vartheta} \frac{u^{\lambda\vartheta-1} - u^{\vartheta-1}}{1-\lambda} = 0, \quad (10)$$

with  $\gamma$  determined a posteriori to impose that  $u^\vartheta$  sums to unity. When  $\lambda \rightarrow 1$ , the limit has to be taken, leading to  $\frac{\gamma}{\vartheta} \frac{u^{\lambda\vartheta-1} - u^{\vartheta-1}}{1-\lambda} \rightarrow \gamma u^{\vartheta-1} \log u$ .

**proof 2** The proof is mainly based on the sharp Gagliardo–Nirenberg inequality [52], as explained with details in Appendix A.

Finally, the minimizers of the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity and the tight bound satisfy a remarkable property of symmetry, as stated hereafter.

**Proposition 3** *Let us consider the involutory transform*

$$\mathfrak{T}_p : (\beta, \lambda) \mapsto \left( \frac{\beta p^* + \lambda - 1}{\lambda p^*}, \frac{1}{\lambda} \right). \quad (11)$$

The minimizers of the complexity satisfy the relation

$$\rho_{p,\mathfrak{T}_p(\beta,\lambda)} \propto \left[ \rho_{p,\beta,\lambda} \right]^\lambda, \quad (12)$$

and the optimal bounds satisfy the relation

$$K_{p,\mathfrak{T}_p(\beta,\lambda)} = \lambda^2 K_{p,\beta,\lambda}. \quad (13)$$

**proof 3** See Appendix B.

A difficulty to determine the sharp bound and the minimizer is to solve the nonlinear differential equation 10. One can find in Corollary 3.2 in [52] a series of explicit equations allowing to determine the solution and thus the optimal bound of in Equation 56, but in general the expression of  $u$  remains on an integral form. Agueh, however, exhibits several situations where the solution is known explicitly (and thus the optimal bound as well), as summarized in the next subsection.

### 2.3 Some Explicitly Known Minimizing Distributions

The particular cases are issued of special cases of saturation of the Gagliardo–Nirenberg, some of them being studied by Bercher [35, 80, 81] or Lutwak [34]. All these cases are restated hereafter, with the notations of the paper. Let us first recall the definition of the stretched deformed Gaussian, studied by Lutwak [34] or Bercher [35, 80, 81], for instance, also known as stretched  $q$ -Gaussian or stretched Tsallis distributions [48, 49] and intensively studied in non-extensive physics.

**Definition 4 (Stretched deformed Gaussian distribution)** Let  $p > 1$  and  $\lambda > 1 - p^*$ . The  $(p, \lambda)$ -stretched deformed Gaussian distribution is defined by

$$g_{p,\lambda}(x) \propto \begin{cases} \left(1 + (1 - \lambda)|x|^{p^*}\right)_+^{\frac{1}{\lambda-1}}, & \text{for } \lambda \neq 1, \\ \exp\left(-|x|^{p^*}\right), & \text{for } \lambda = 1, \end{cases} \quad (14)$$

where  $(\cdot)_+ = \max(\cdot, 0)$  (the case  $\lambda = 1$  is indeed obtained taking the limit).

This distribution plays a fundamental role in the extended Stam inequality, as we will see in the next subsections and in the next section.

#### 2.3.1 The Case $\beta = \lambda$

For any  $p > 1$ , and for

$$(\beta, \lambda) \in \mathcal{B}_p = \{(\beta, \lambda) \in \mathcal{D}_p : \beta = \lambda\}, \quad (15)$$

one obtains that the minimizing distribution of the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity is the  $(p, \lambda)$ -stretched deformed Gaussian distribution,

$$\rho_{p,\lambda,\lambda} = g_{p,\lambda} \quad (16)$$

(see Corollary 3.4 in [52], (i) where  $\lambda = q/s$ ; and (ii) where  $\lambda = s/q$ , respectively; the case  $\lambda = 1$  is obtained taking the limit  $\lambda \rightarrow 1$  (resp. lower and upper limit) or by a direct computation). This situation is nothing more than that studied by Bercher in [35] or Lutwak in [34]. Remarkably, by a mass transport approach, Lutwak proved in [34] that this relation is valid for  $\lambda > \frac{1}{1+p^*}$ , i.e., for

$$(\beta, \lambda) \in \mathcal{L}_p = \left\{ (\beta, \lambda) \in \mathbb{R}_+^{*2} : \beta = \lambda > \frac{1}{1+p^*} \right\}. \quad (17)$$

Note that the exponent of the Lutwak expression is not the same as ours, but  $\beta > 0$  allowing to take the Lutwak relation to the adequate exponent so as to obtain our formulation.

### 2.3.2 Stretched Deformed Gaussian: The Symmetric Case

Immediately, from the relation Equation 12 induced by the involution  $\mathfrak{T}_p$ , one obtains, after a re-parametrization  $\lambda \mapsto \frac{1}{\lambda}$  and an adequate scaling, for any  $p > 1$  and

$$(\beta, \lambda) \in \overline{\mathcal{B}}_p = \left\{ (\beta, \lambda) \in \mathcal{D}_p : \beta = \frac{p^* + 1 - \lambda}{p^*} \right\} \quad (18)$$

that the minimizing distribution is again a stretched deformed Gaussian,

$$\rho_{p, \frac{p^*+1-\lambda}{p^*}, \lambda} = g_{p, 2-\lambda}. \quad (19)$$

Again, starting from the Lutwak result, the validity of this result extends to

$$(\beta, \lambda) \in \overline{\mathcal{L}}_p = \left\{ (\beta, \lambda) \in \mathbb{R}_+^{*2} : 0 < \beta = \frac{p^* + 1 - \lambda}{p^*} < 1 + \frac{1}{p^*} \right\}, \quad (20)$$

and the symmetry of the bound given by Proposition 3 remains valid. Indeed, the minimizers in  $\mathcal{L}_p$  satisfying the differential equation of the Gagliardo–Nirenberg as given in Appendix A, the reasoning of this appendix and of the Appendix B holds.

### 2.3.3 Dealing with the Usual Fisher Information

This situation corresponds to  $p = 2$  and  $\beta = 1$ . Then, for

$$(\beta, \lambda) \in \mathcal{A}_2 = \{(\beta, \lambda) \in \mathcal{D}_2 : \beta = 1\}, \quad (21)$$

one obtains the minimizing distribution for  $\lambda \neq 1$ ,

$$\rho_{2,1,\lambda}(x) \propto \left[ \cos \left( \sqrt{1-\lambda} |x| \right) \right]^{\frac{2}{1-\lambda}} \mathbb{1}_{\left[0; \frac{\pi}{2\Re\{\sqrt{1-\lambda}\}}\right)}(|x|), \quad (22)$$

where  $\mathbb{1}_A$  denotes the indicator function of set  $A$ ,  $\sqrt{-1} = i$  (remember that  $\cos(ix) = \cosh(x)$ ),  $\Re$  is the real part and  $\frac{1}{0}$  is to be understood as  $+\infty$  (see Corollary 3.3 in [51] with  $\lambda = s/q$  and Corollary 3.4 in [51] with  $\lambda = q/s$ , respectively). The case  $\lambda = 1$  is again obtained by taking the limit, leading to the Gaussian distribution  $\rho_{2,1,1}$ . (See previous cases, with  $p = 2$ , that corresponds also to the usual Stam inequality.)

### 2.3.4 The Symmetrical of the Usual Fisher Information

From the relation Equation 12 induced by the involution  $\mathfrak{F}_p$ , after a re-parametrization  $\lambda \mapsto \frac{1}{\lambda}$  and an adequate scaling, for  $p = 2$  and

$$(\beta, \lambda) \in \overline{\mathcal{A}}_2 = \left\{ (\beta, \lambda) \in \mathcal{D}_2 : \beta = \frac{\lambda+1}{2} \right\}, \quad (23)$$

the minimizing distribution for  $\lambda \neq 1$  takes the form

$$\rho_{2, \frac{\lambda+1}{2}, \lambda}(x) \propto \left[ \cos \left( \sqrt{\lambda-1} |x| \right) \right]^{\frac{2}{\lambda-1}} \mathbb{1}_{\left[0; \frac{\pi}{2\Re\{\sqrt{\lambda-1}\}}\right)}(|x|) \quad (24)$$

(with, again, the Gaussian as the limit when  $\lambda \rightarrow 1$ ).

The graphs in Figure 1 describe the domain  $\mathcal{D}_p$  (for a given  $p$ ). Therein, we also represent the particular domains  $\mathcal{L}_p$  (Bercher–Lutwak situation),  $\overline{\mathcal{L}}_p$  (transformation of  $\mathcal{L}_p$ ),  $\mathcal{A}_2$  and  $\overline{\mathcal{A}}_2$ , where the explicit expressions of the minimizing distributions are known from the works of [51, 52, 34, 35].

## 3 Extended Optimal Stam Inequality: A Step Further

In this section, we further extend the previous Stam inequality, namely by largely widening the domain for the parameters and disentangling the two connected parameters. For this, we use the *differential-escort deformation* introduced in [50], which is the key tool allowing for introducing a new degree of freedom. Afterwards, we will give the minimizing distribution that results in a new deformation of the Gaussian family intimately linked with the inverse incomplete beta functions.

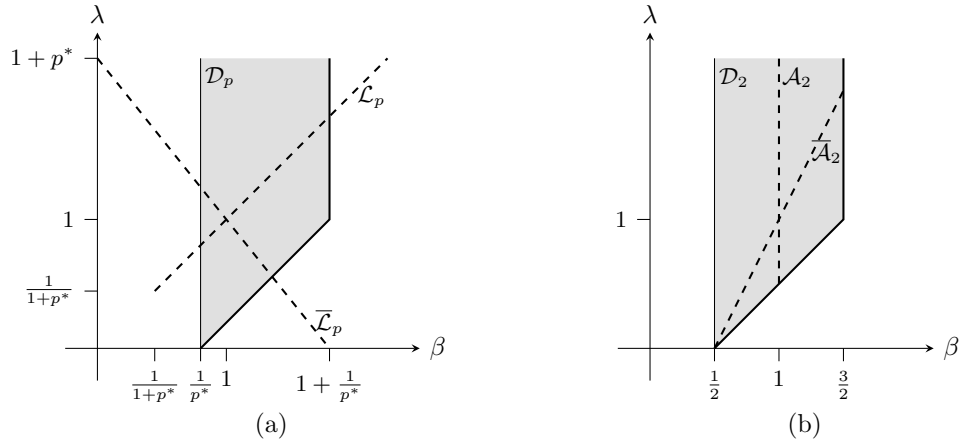


Figure 1: (a) the domain  $\mathcal{D}_p$  for a given  $p$  is represented by the gray area (here  $p > 2$ ). The thick line belongs to  $\mathcal{D}_p$ . The dashed line represents  $\mathcal{L}_p$ , corresponding to the Lutwak situation of Section 2.3.1, where the relation holds and the minimizers are explicitly known (stretched deformed Gaussian distributions), whereas  $\bar{\mathcal{L}}_p$  corresponds to Section 2.3.2 ( $\mathcal{B}_p$  and  $\bar{\mathcal{B}}_p$  obtained by the Gagliardo–Nirenberg inequality are their restrictions to  $\mathcal{D}_p$ ); (b) same situation for  $p = 2$ , with the domains  $\mathcal{A}_2$  and  $\bar{\mathcal{A}}_2$  (dashed lines) that correspond to the situations of Sections 2.3.3 and 2.3.4, respectively, ( $\mathcal{L}_2$  and  $\bar{\mathcal{L}}_2$  are not represented for the clarity of the figure).

### 3.1 Differential-Escort Distribution: A Brief Overview

We have already realized the crucial role that the power operation of a probability density function  $\rho$  plays. The subsequent escort distribution duly normalized,  $\frac{\rho(x)^\alpha}{\int_{\mathbb{R}} \rho(x)^\alpha dx}$ , is a simple monoparametric deformation of  $\rho$  (see e.g., [82]). Notice that the parameter  $\alpha$  allows us to explore different regions of  $\rho$ , so that, for  $\alpha > 1$ , the more singular regions are amplified and, for  $\alpha < 1$ , the less singular regions are magnified. A careful look at the minimizing distributions of the usual Stam inequality shows that the  $x$ -axis is stretched via a power operation. This makes us guess that a certain nonlinear stretching may also play a key role in the saturation (i.e., equality) of the extended Stam inequality.



These ideas led us to the definition of the differential-escort distribution of a probability distribution  $\rho$  (see also [50]), motivated by the following principle. The power operation provokes a two-fold stretching in the density itself and in the differential interval so as to conserve the probability in the differential intervals:  $\rho_\alpha(y)dy = \rho(x)dx$  with  $\rho_\alpha(y) = \rho(x(y))^\alpha$ .

**Definition 5 (Differential-escort distributions)** *Given a probability distribution  $\rho(x)$  and given an index  $\alpha \in \mathbb{R}$ , the differential-escort distribution of  $\rho$  of order  $\alpha$  is defined as*

$$\mathfrak{E}_\alpha[\rho](y) = \left[ \rho(x(y)) \right]^\alpha, \tag{25}$$

where  $y(x)$  is a bijection satisfying  $\frac{dy}{dx} = [\rho(x)]^{1-\alpha}$  and  $y(0) = 0$ .

The differential-escort transformation  $\mathfrak{E}_\alpha$  exhibits various properties studied in detail in [50]. We present here the key ones, allowing the extension of the Stam inequality in a wider domain than that of the previous section.

**Property 1** *The differential-escort transformation satisfies the composition relation*

$$\mathfrak{E}_\alpha \circ \mathfrak{E}_{\alpha'} = \mathfrak{E}_{\alpha'} \circ \mathfrak{E}_\alpha = \mathfrak{E}_{\alpha\alpha'} \tag{26}$$

where  $\circ$  is the composition operator. Moreover, since  $\mathfrak{E}_1$  is the identity, for any  $\alpha \neq 0$ ,  $\mathfrak{E}_\alpha$  is invertible and,

$$\mathfrak{E}_\alpha^{-1} = \mathfrak{E}_{\alpha^{-1}}. \tag{27}$$

In addition to the trivial case  $\alpha = 1$ , keeping invariant the distribution, a remarkable case is given by  $\alpha = 0$ , leading to the uniform distribution. This case is non surprising since then  $x(y)$  is nothing more than the inverse of the cumulative density function, well known to uniformize a random vector [83].

In the sequel, we focus on the differential-escort distributions obtained for  $\alpha > 0$ . Under this condition, when  $\rho$  is continuously differentiable, its differential-escort is also continuously differentiable. This is important to be able to define its  $(p, \lambda)$ -Fisher information (see Definition 2). Under this condition, the differential-escort transformation induces a scaling property on the index of the Rényi entropy power (for this quantity it remains true for any  $\alpha \in \mathbb{R}$ ), the  $(p, \beta)$ -Fisher information, and thus on the subsequent complexity as stated in the following proposition.

**Proposition 4** *Let a probability distribution  $\rho$  and an index  $\alpha > 0$ . Then, the Rényi entropy powers of  $\rho$  and its differential-escort distribution  $\mathfrak{E}_\alpha[\rho]$  satisfy that*

$$N_\lambda[\mathfrak{E}_\alpha[\rho]] = \left(N_{1+\alpha(\lambda-1)}[\rho]\right)^\alpha \quad (28)$$

for any  $\lambda \in \mathbb{R}_+^*$ . Moreover, if the density  $\rho$  is continuously differentiable, then the extended Fisher information of  $\rho$  and its differential-escort distribution  $\mathfrak{E}_\alpha[\rho]$  satisfy that

$$F_{p,\beta}[\mathfrak{E}_\alpha[\rho]] = \alpha^{\frac{2}{\beta}} \left(F_{p,\alpha\beta}[\rho]\right)^\alpha \quad (29)$$

for any  $p > 1, \beta \in \mathbb{R}_+^*$ .

Consequently, the  $(p, \beta, \lambda)$ -Fisher-Rényi complexity of  $\rho$  and of  $\mathfrak{E}_\alpha[\rho]$  satisfy the relation

$$C_{p,\beta,\lambda}[\mathfrak{E}_\alpha[\rho]] = \alpha^2 C_{p,\mathfrak{A}_\alpha(\beta,\lambda)}[\rho]. \quad (30)$$

**proof 4** *It is straightforward to note that*

$$\begin{aligned} \left(N_\lambda[\mathfrak{E}_\alpha[\rho]]\right)^{\frac{1-\lambda}{2}} &= \int_{\mathbb{R}} [\mathfrak{E}_\alpha[\rho](y)]^\lambda dy \\ &= \int_{\mathbb{R}} [\mathfrak{E}_\alpha[\rho](y(x))]^\lambda \frac{dy}{dx} dx \\ &= \int_{\mathbb{R}} [\rho(x)]^{\alpha\lambda+1-\alpha} dx \\ &= \left(N_{1+\alpha(\lambda-1)}[\rho]\right)^{\frac{\alpha(1-\lambda)}{2}}, \end{aligned}$$

leading to Equation 28.

Similarly,

$$\begin{aligned} \left(F_{p,\beta}[\mathfrak{E}_\alpha[\rho]]\right)^{\frac{p\beta}{2}} &= \int_{\mathbb{R}} \left| [\mathfrak{E}_\alpha[\rho](y)]^{\beta-2} \frac{d}{dy} [\mathfrak{E}_\alpha[\rho](y)] \right|^p \mathfrak{E}_\alpha[\rho](y) dy \\ &= \int_{\mathbb{R}} \left| [\mathfrak{E}_\alpha[\rho](y(x))]^{\beta-2} \frac{d}{dx} [\mathfrak{E}_\alpha[\rho](y(x))] \frac{dx}{dy} \right|^p \mathfrak{E}_\alpha[\rho](y(x)) \frac{dy}{dx} dx \\ &= \int_{\mathbb{R}} \left| [\rho(x)]^{\alpha(\beta-2)} \frac{d}{dx} [(\rho(x))^\alpha] [\rho(x)]^{\alpha-1} \right|^p \rho(x) dx \\ &= \int_{\mathbb{R}} \left| \alpha [\rho(x)]^{\alpha\beta-2} \frac{d}{dx} [\rho(x)] \right|^p \rho(x) dx, \end{aligned}$$

leading to Equation 29.

Relation 30 is a consequence of Equations 28 and 29 together with Definition 3 of the complexity.

One may mention [84] where the author studies the effect of a rescaling of the Tsallis non-additive parameter, equivalent to the entropic parameter of the Rényi entropy, and that is exactly that of Equation 28. In particular, this rescaling has an effect on the maximum entropy distribution in such a way that it is equivalent to elevate this particular distribution to a power. Here, the spirit is slightly different since we start from a given distribution and the nonlinear stretching is made on the state ( $x$ -axis) of any probability density in such a way that it is elevated to an exponent. The stretching is intimately linked to the distribution, being of maximum entropy or not, and the scaling effect on the Rényi is a consequence of this nonlinear stretching. The study of the links between the present result and that of [84] goes beyond the scope of our work and remains as a perspective.

### 3.2 Enlarging the Validity Domain of the Extended Stam Inequality

We have now all the ingredients to enlarge the domain of validity of the Stam inequality. Moreover, we are able to determine an explicit expression of the minimizer by the mean of a special function, i.e., more simple to determine than as in Proposition 2, and of the tight bound as well.

To this aim, let us consider the following affine transform  $\mathfrak{A}_a$  and the set of transformation for  $a \in \mathbb{R}_+^*$ ,

$$\mathfrak{A}_a : (\beta, \lambda) \mapsto (a\beta, 1+a(\lambda-1)) \quad \text{and} \quad \mathfrak{A}(\beta, \lambda) = \{\mathfrak{A}_a(\beta, \lambda) : a \in \mathbb{R}_+^*\} \cap \mathbb{R}_+^{*2}. \quad (31)$$

Then, for any strictly positive real  $a$ , one can apply Proposition 2 to  $\mathfrak{E}_a[\rho]$ , that is, for  $p > 1$ ,  $(\beta, \lambda) \in \mathcal{D}_p$ ,  $C_{p,\beta,\lambda}[\mathfrak{E}_a[\rho]] \geq K_{p,\beta,\lambda}$ . Thus, from Proposition 4, one immediately has that  $C_{p,\mathfrak{A}_a(\beta,\lambda)}[\rho] \geq a^{-2}K_{p,\beta,\lambda} \equiv K_{p,\mathfrak{A}_a(\beta,\lambda)}$ . Moreover, this inequality is sharp since it is achieved for  $\mathfrak{E}_a[\rho] = \rho_{p,\beta,\lambda}$ , i.e., for  $\rho_{p,\mathfrak{A}_a(\beta,\lambda)} = \mathfrak{E}_{a^{-1}}[\rho_{p,\beta,\lambda}]$ .

As a conclusion, the existence of a universal optimal positive constant bounding the complexity (see Proposition 2) extends from  $\mathcal{D}_p$  to  $\mathfrak{A}(\mathcal{D}_p)$ . Note that  $\mathfrak{A}(\beta, \lambda)$  is the overlap of the line defined by the point  $(0, 1)$  and  $(\beta, \lambda)$  itself (achieved for  $a = 1$ ), and  $\mathbb{R}_+^{*2}$ , as depicted Figure 2. Then, it is straightforward to see that  $\tilde{\mathcal{D}}_p \equiv \mathfrak{A}(\mathcal{D}_p) = \{(\beta, \lambda) \in \mathbb{R}_+^{*2} : \lambda > 1 - \beta p^*\}$  (see Figure 2a). The approach is thus the following:

- Consider a point  $(\beta, \lambda) \in \widetilde{\mathcal{D}}_p$  and find an index  $\alpha \in \mathbb{R}_+^*$  such that  $\mathfrak{A}_\alpha(\beta, \lambda) \in \mathcal{D}_p$ , which is a point of the intersection between  $\mathcal{D}_p$  and the line joining  $(0, 1)$  and  $(\beta, \lambda)$ .
- Apply Proposition 2 for the point  $(p, \mathfrak{A}_\alpha(\beta, \lambda))$ , leading to the minimizing distribution  $\rho_{p, \mathfrak{A}_\alpha(\beta, \lambda)}$  and its corresponding bound.
- Then, remarking that  $\mathfrak{A}_{\alpha^{-1}} \circ \mathfrak{A}_\alpha(\beta, \lambda) = (\beta, \lambda)$ , the minimizer of the extended complexity writes  $\rho_{p, \beta, \lambda} = \mathfrak{E}_\alpha \left[ \rho_{p, \mathfrak{A}_\alpha(\beta, \lambda)} \right]$  and the corresponding bound can be computed from this minimizer or noting that  $K_{p, \beta, \lambda} = \alpha^2 K_{p, \mathfrak{A}_\alpha(\beta, \lambda)}$ .

The same procedure obviously applies dealing with  $\mathcal{L}_p$ :  $\mathfrak{A}(\mathcal{L}_p) = \{(\beta, \lambda) \in \mathbb{R}_+^{*2} : 1 - \beta p^* < \lambda < \beta + 1\}$  appears to be a subset of  $\widetilde{\mathcal{D}}_p$  (see Figure 2b). Similarly, one can also deal with  $\overline{\mathcal{L}}_p$ :  $\mathfrak{A}(\overline{\mathcal{L}}_p) = \{(\beta, \lambda) \in \mathbb{R}_+^{*2} : \lambda > 1 - \frac{p^* \beta}{p^* + 1}\}$  also appears to be a subset of  $\widetilde{\mathcal{D}}_p$  (see Figure 2c). Remarkably,  $\mathfrak{A}(\mathcal{D}_p) = \mathfrak{A}(\mathcal{L}_p) \cup \mathfrak{A}(\overline{\mathcal{L}}_p)$ . Moreover, we have explicit expressions for the minimizers in both  $\mathcal{L}_p$  and  $\overline{\mathcal{L}}_p$ , which greatly eases determining the minimizers in  $\widetilde{\mathcal{D}}_p$  (including  $\mathcal{D}_p$  itself).

These remarks, together with both the knowledge of the minimizing distributions and the bound on  $\mathcal{L}_p \cup \overline{\mathcal{L}}_p$ , lead to the following definition and proposition.

**Definition 6 (( $p, \beta, \lambda$ )-Gaussian distribution)** For any  $p > 1$  and  $(\beta, \lambda) \in \mathbb{R}_+^{*2}$ , we define the ( $p, \beta, \lambda$ )-Gaussian distribution as

$$g_{p, \beta, \lambda}(x) \propto \begin{cases} \left[ 1 - \mathfrak{B}^{-1} \left( \frac{1}{p^*}, q_{p, \beta, \lambda}; \frac{p^* |x|}{|1 - \lambda| p^*} \right) \right]^{\frac{1}{|1 - \lambda|}} \mathbb{1}_{\left[0; B \left( \frac{1}{p^*}, q_{p, \beta, \lambda} \right)\right]} \left( \frac{p^* |x|}{|1 - \lambda| p^*} \right), & \text{if } \lambda \neq 1, \\ \exp \left( - \frac{\mathfrak{E}^{-1} \left( \frac{1}{p^*}; \left( \frac{\beta - 1}{\beta} \right)^{\frac{1}{p^*}} p^* |x| \right)}{\beta - 1} \right) \mathbb{1}_{\left[0; \frac{\Gamma(1/p^*)}{\frac{1}{1} (0; 1)^{(\beta)}}\right]} (p^* |x|), & \text{if } \begin{matrix} \lambda = 1, \\ \beta \neq 1, \end{matrix} \\ \exp(-|x|^{p^*}), & \text{if } \beta = \lambda = 1, \end{cases} \quad (32)$$

with

$$q_{p, \beta, \lambda} = \frac{\beta - 1}{|1 - \lambda|} + \frac{\mathbb{1}_{\mathbb{R}_+}(1 - \lambda)}{p}. \quad (33)$$

$\mathfrak{T}_p$  is the involutory transform defined Equation 11.  $\mathfrak{B}(a, b, x) = \int_0^x t^{a-1} (1-t)^{b-1} dt$  is the incomplete beta function, defined when  $a > 0$  and for  $x \in [0; 1)$

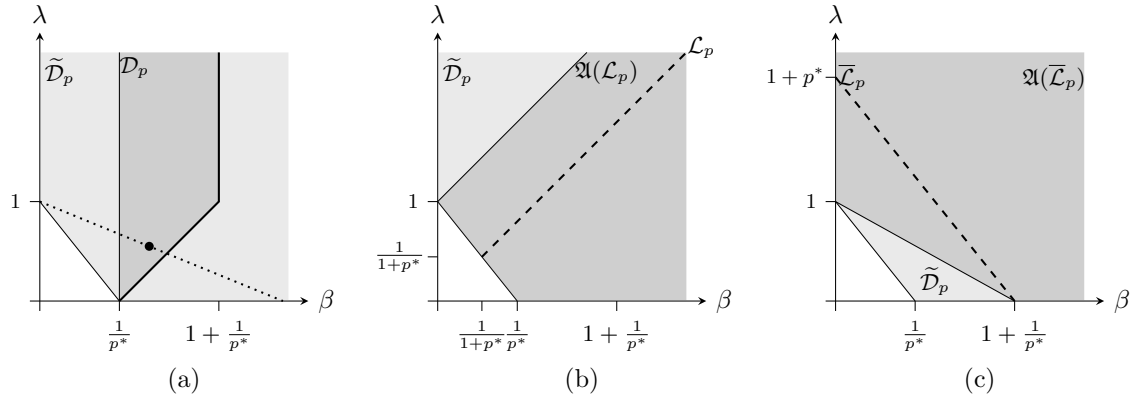


Figure 2: Given a  $p$ , the domain in gray represents  $\tilde{\mathcal{D}}_p$ , where we know that the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity is optimally lower bounded and where the minimizers can be deduced from proposition 2. (a) the domain in dark gray represents  $\mathcal{D}_p$ , which is obviously included in  $\tilde{\mathcal{D}}_p$ ; the dot is a particular point  $(\beta, \lambda) \in \mathcal{D}_p$  and the dotted line represents its transform by  $\mathfrak{A}$ ; (b) the domain in dark gray represents  $\mathfrak{A}(\mathcal{L}_p) \subset \tilde{\mathcal{D}}_p$ , which obviously contains  $\mathcal{L}_p$  represented by the dashed line; (c) same as (b) with  $\bar{\mathcal{L}}_p$  and  $\mathfrak{A}(\bar{\mathcal{L}}_p) \subset \tilde{\mathcal{D}}_p$ . This illustrates that  $\tilde{\mathcal{D}}_p = \mathfrak{A}(\mathcal{L}_p) \cup \mathfrak{A}(\bar{\mathcal{L}}_p)$ .

(see [85]), and  $B(a, b) = \lim_{x \rightarrow 1} \mathfrak{B}(a, b, x)$ , that is the standard beta function if  $b > 0$  and infinite otherwise.  $\mathfrak{B}^{-1}$  is thus the inverse incomplete beta function. Finally,  $\mathfrak{G}(a, x) = \int_0^x t^{a-1} \exp(-t) dt$  is the incomplete gamma function, defined when  $a > 0$  and for  $x \in \mathbb{R}$  [85], and  $\Gamma(a) = \lim_{x \rightarrow +\infty} \mathfrak{G}(a, x)$  is the gamma function. By definition,  $z^\alpha = |z|^\alpha e^{i\alpha \text{Arg}(t)}$  where  $0 \leq \text{Arg}(t) < 2\pi$ . Finally, by convention  $1/0 = +\infty$ .

Note that, when  $b > 0$ , the inverse incomplete beta function is well known and tabulated in the usual mathematical softwares since it is the inverse cumulative function of the beta distributions [86]. Otherwise, as the incomplete beta function writes through an hypergeometric function [87] (see also [85, 86]), also well known and tabulated,  $\mathfrak{B}^{-1}$  can be at least numerically computed. The incomplete beta function contains many special cases for particular parameters [87, 88]. For instance, when  $a + b$  is a negative

integer, they express as elementary functions [87].

Similarly, when its argument is positive, the incomplete gamma function and its inverse are well known and tabulated because they are linked to the cumulative distribution of gamma laws [86]. Even for negative arguments, the incomplete gamma function is very often tabulated in mathematical software. Otherwise, one can write it using a confluent hypergeometric function [85] (see also [87, 86]), generally tabulated. Thus, it can be inverted at least numerically. The incomplete gamma function also contains special cases for particular parameters. For instance,  $\mathfrak{G}\left(\frac{1}{2}, x^2\right) = \text{erf}(x)$ , where erf is the error function [85]. Hence, for  $p = 2$  and  $\lambda = 1$ , the  $(p, \beta, \lambda)$ -Gaussian writes in terms of the inverse error function.

Now, from the procedure previously described, we obtain the Stam inequality with the widest possible domain, together with the minimizing distributions and the explicit tight lower bound.

**Proposition 5 (Stam inequality in a wider domain)** *The  $(p, \beta, \lambda)$ -Fisher-Rényi complexity is non trivially lower bounded as follows:*

$$\forall p > 1, \quad (\beta, \lambda) \in \tilde{\mathcal{D}}_p = \{(\beta, \lambda) \in \mathbb{R}_+^{*2} : \lambda > 1 - \beta p^*\}, \quad C_{p,\beta,\lambda}[\rho] \geq K_{p,\beta,\lambda}. \quad (34)$$

The minimizers are explicitly given by

$$\text{argmin}_\rho C_{p,\beta,\lambda}[\rho] = g_{p,\beta,\lambda}, \quad (35)$$

the  $(p, \beta, \lambda)$ -Gaussian of Definition 6. Proposition 3 remains valid in  $\tilde{\mathcal{D}}_p$ . Moreover, the tight bound is

$$K_{p,\beta,\lambda} = \begin{cases} \left( \frac{2}{p^* \zeta_{p,\beta,\lambda}} \left( \frac{p^* \zeta_{p,\beta,\lambda}}{|1-\lambda|} \right)^{\frac{1}{p^*}} \left( \frac{p^* \zeta_{p,\beta,\lambda}}{p^* \zeta_{p,\beta,\lambda} - |1-\lambda|} \right)^{\frac{\zeta_{p,\beta,\lambda}}{|1-\lambda|} + \frac{1}{p}} B\left(\frac{1}{p^*}, \frac{\zeta_{p,\beta,\lambda}}{|1-\lambda|} + \frac{1}{p}\right) \right)^2, & \text{if } \lambda \neq 1, \\ \left( \frac{2 e^{\frac{1}{p^*}} \Gamma\left(\frac{1}{p^*}\right)}{\beta p^* \frac{1}{p}} \right)^2, & \text{if } \lambda = 1, \end{cases} \quad (36)$$

with

$$\zeta_{p,\beta,\lambda} = \beta + \frac{(\lambda - 1)_+}{p^*}. \quad (37)$$

**proof 5** See Appendix C.

## 4 Applications to Quantum Physics

Let us now apply the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity for some specific values of the parameters to the analysis of the two main prototypes of  $d$ -dimensional quantum systems subject to a central (i.e., spherically symmetric) potential; namely, the hydrogenic and harmonic (i.e., oscillator-like) systems. The wave functions of the bound stationary states of these systems have the same angular part, so that we concentrate here on the radial distribution in both position and momentum spaces.

### 4.1 Brief Review on the Quantum Systems with Radial Potential

The time-independent Schrödinger equation of a single-particle system in a central potential  $V(r)$  can be written as

$$\left(-\frac{1}{2}\vec{\nabla}_d^2 + V(r)\right)\Psi(\vec{r}) = E_n \Psi(\vec{r}), \quad (38)$$

(atomic units are used from here onwards), where  $\vec{\nabla}_d$  denotes the  $d$ -dimensional gradient operator and the position vector  $\vec{r} = (x_1, \dots, x_d)$  in hyperspherical units is given by  $(r, \theta_1, \theta_2, \dots, \theta_{d-1}) \equiv (r, \Omega_{d-1})$ ,  $\Omega_{d-1} \in \mathbb{S}^{d-1}$  the unit  $d$ -dimensional sphere, where  $r \equiv |\vec{r}| = \sqrt{\sum_{i=1}^d x_i^2} \in \mathbb{R}_+$  and  $x_i = r \left(\prod_{k=1}^{i-1} \sin \theta_k\right) \cos \theta_i$  for  $1 \leq i \leq d$  and with  $\theta_i \in [0; \pi)$  for  $i < d-1$ ,  $\theta_{d-1} \equiv \phi \in [0; 2\pi)$  and  $\theta_d = 0$  by convention. The physical wave functions are known to factorize (see e.g., [89, 90, 91]) as

$$\Psi_{n,l,\{\mu\}}(\vec{r}) = \mathcal{R}_{n,l}(r) \mathcal{Y}_{l,\{\mu\}}(\Omega_{d-1}), \quad (39)$$

where  $\mathcal{R}_{n,l}(r)$  and  $\mathcal{Y}_{l,\{\mu\}}(\Omega_{d-1})$  denote the radial and the angular part, respectively, being  $(l, \{\mu\}) \equiv (l \equiv \mu_1, \mu_2, \dots, \mu_{d-1})$  the hyperquantum numbers associated to the angular variables  $\Omega_{d-1} \equiv (\theta_1, \theta_2, \dots, \theta_{d-1})$ , which may take all values consistent with the inequalities  $l \equiv \mu_1 \geq \mu_2 \geq \dots \geq |\mu_{d-1}| \equiv |m| \geq 0$ .

As already stated, the angular part  $\mathcal{Y}_{l,\{\mu\}}$  is independent of the potential  $V$  and its expression is detailed in [91, 14, 92, 17], for instance. Only the radial part  $\mathcal{R}_{n,l}$  is dependent on  $V$  (and also on the energy level  $n$  and the angular quantum number  $l$ ), being the solution of the radial differential

equation

$$\left( -\frac{1}{2} \frac{d^2}{dr^2} - \frac{d-1}{2r} \frac{d}{dr} + \frac{l(l+d-2)}{2r^2} + V(r) \right) \mathcal{R}_{n,l}(r) = E_n \mathcal{R}_{n,l}(r) \quad (40)$$

(see e.g., [14, 92, 17] for further details). Then, the associated radial probability density  $\rho(r)$  is given by

$$\rho_{n,l}(r) dr = \int_{\mathbb{S}^{d-1}} |\Psi(\vec{r})|^2 d\vec{r} = [\mathcal{R}_{n,l}(r)]^2 r^{d-1} dr, \quad (41)$$

where we have taken into account the volume element  $d\vec{r} = r^{d-1} dr d\Omega_{d-1}$  and the normalization of the hyperspherical harmonics  $\mathcal{Y}_{l,\{\mu\}}(\Omega_{d-1})$  to unity.

Then, the wavefunction associated to the momentum of the system is given by the Fourier transform  $\tilde{\Psi}$  of  $\Psi$ . It is known that, again,  $\tilde{\Psi}$  writes as the product of a radial and angular part

$$\tilde{\Psi}_{n,l,\{\mu\}}(\vec{k}) = \mathcal{M}_{n,l}(k) \mathcal{Y}_{l,\{\mu\}}(\Omega_{d-1}), \quad (42)$$

with the radial part being the modified Hankel transform of  $\mathcal{R}_{n,l}$ ,

$$\mathcal{M}_{n,l}(k) = (-i)^l k^{1-\frac{d}{2}} \int_{\mathbb{R}_+} r^{\frac{d}{2}} \mathcal{R}_{n,l}(r) J_{l+\frac{d}{2}-1}(kr) dr, \quad (43)$$

with  $J_\nu$  the Bessel function of the first kind and order  $\nu$  (see e.g., [91, 14, 92, 17]). Again, it leads to the radial probability density function

$$\gamma_{n,l}(k) = [\mathcal{M}_{n,l}(k)]^2 k^{d-1}. \quad (44)$$

In the following, we will focus on the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity of the radial densities  $\rho_{n,l}(r)$  and  $\gamma_{n,l}(k)$  of the  $d$ -dimensional harmonic and hydrogenic systems.

#### 4.2 $(p, \beta, \lambda)$ -Fisher–Rényi Complexity and the Hydrogenic System

The bound states of a  $d$ -dimensional hydrogenic system, where  $V(r) = -\frac{Z}{r}$  ( $Z$  denotes the nuclear charge) are the physical solutions of Equation 40, which correspond to the known energies

$$E_n^{(h)} = -\frac{Z^2}{2\eta^2} \quad \text{where} \quad \eta = n + \frac{d-3}{2}; \quad n = 1, 2, \dots \quad (45)$$



(see [89, 90, 14]). The radial eigenfunctions are given by

$$\mathcal{R}_{n,l}^{(h)}(r) = \sqrt{R_{n,l}} \left(\frac{2Z}{\eta}\right)^{\frac{d-1}{2}} \tilde{r}^l e^{-\frac{\tilde{r}}{2}} \mathcal{L}_{\eta-L-1}^{(2L+1)}(\tilde{r}). \quad (46)$$

$L$  is the *grand* orbital angular momentum quantum number,  $\tilde{r}$  is a dimensionless parameter, and the normalization coefficient  $R_{n,l}$  are given by

$$L = l + \frac{d-3}{2}, \quad l = 0, 1, \dots, n-1; \quad \tilde{r} = \frac{2Z}{\eta} r \quad \text{and} \quad R_{n,l} = \frac{Z \Gamma(\eta - L)}{\eta^2 \Gamma(\eta + L + L)}, \quad (47)$$

respectively, with  $\mathcal{L}_n^{(\alpha)}(x)$  the Laguerre polynomials [85, 87]. Then, the radial probability density (41) of a  $d$ -dimensional hydrogenic stationary state  $(n, l, \{\mu\})$  is given in position space by

$$\rho_{n,l}^{(h)}(r) = R_{n,l} \tilde{r}^{2L+2} e^{-\tilde{r}} \left[\mathcal{L}_{\eta-L-1}^{(2L+1)}(\tilde{r})\right]^2. \quad (48)$$

Furthermore, using 8.971 in [87], one can compute  $\frac{d\rho_{n,l}^{(h)}}{dr} = \frac{2Z}{\eta} \frac{d\rho_{n,l}^{(h)}}{d\tilde{r}}$ .

On the other hand, the modified Hankel transform of  $\mathcal{R}_{n,l}$  Equation 43 gives the radial part of the wavefunction in the conjugated momentum space as [89, 90, 14]

$$\mathcal{M}_{n,l}(k) = \sqrt{M_{n,l}} \left(\frac{\eta}{Z}\right)^{\frac{d-1}{2}} \frac{\tilde{k}^l}{(1 + \tilde{k}^2)^{L+2}} \mathcal{G}_{\eta-L-1}^{(L+1)}\left(\frac{1 - \tilde{k}^2}{1 + \tilde{k}^2}\right), \quad (49)$$

where  $\tilde{k}$  is a dimensionless parameter and the normalization coefficient  $M_{n,l}$  are given by

$$\tilde{k} = \frac{\eta}{Z} k \quad \text{and} \quad M_{n,l} = \frac{4^{2L+3} \Gamma(\eta - L) [\Gamma(L + 1)]^2 \eta^2}{2 \pi Z \Gamma(\eta + L + 1)}, \quad (50)$$

and where  $\mathcal{G}_n^{(\alpha)}(x)$  denotes the Gegenbauer polynomials [85, 87]. This gives the radial probability density function in the momentum space as

$$\gamma_{n,l}^{(h)}(k) = M_{n,l} \frac{\tilde{k}^{2L+2}}{(1 + \tilde{k}^2)^{2L+4}} \left[\mathcal{G}_{\eta-L-1}^{(L+1)}\left(\frac{1 - \tilde{k}^2}{1 + \tilde{k}^2}\right)\right]^2. \quad (51)$$

Furthermore, using 8.939 in [87], one can compute  $\frac{d\gamma_{n,l}^{(h)}}{dk} = \frac{2Z}{\eta} \frac{d\gamma_{n,l}^{(h)}}{d\tilde{k}}$ .

These expressions can thus be injected into Equations 4–6 to evaluate the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity of both  $\rho_{n,l}^{(h)}$  and  $\gamma_{n,l}^{(h)}$ . Due to the special form of the density, involving orthogonal polynomials, this can be done using for instance a Gauss-quadrature method for the integrations [86].

For illustration purposes, we depict in Figure 3 the behavior of the Fisher information  $F_{p,\beta}$ , of the Rényi entropy power  $N_\lambda$ , and of the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity  $C_{p,\beta,\lambda}$  (normalized by the lower bound) of the radial position density  $\rho_{n,l}^{(h)}$  of the  $d$ -dimensional hydrogenic system, versus  $n$  and  $l$ , for the parameters  $(p, \beta, \lambda) = (2, 1, 7)$  and in dimensions  $d = 3$  and  $12$ . Therein, we firstly observe that, for a given quantum state of the system (so, when  $n$  and  $l$  are fixed), the Fisher information decreases (see left graph) and the Rényi entropy power increases (see center graph) when  $d$  goes from 3 to 12. This indicates that the oscillatory degree and the spreading amount of the radial electron distribution have a decreasing and increasing behavior, respectively, when the dimension is increasing. The resulting combined effect, as captured and quantified by the the Fisher–Rényi complexity (see right graph), is such that the complexity has a clear dependence on the difference  $n - l$  in such a delicate way that it decreases when  $n - l = 1$ , but it increases when  $n - l$  is bigger than unity as  $d$  is increasing.

To better understand this phenomenon, we have to look carefully at the opposite behavior of the Fisher information and the Rényi entropy power versus the pair  $(n, l)$ .

Indeed, for the two dimensionality cases considered in this work, the Fisher information presents a decreasing behavior when  $l$  is increasing and  $n$  is fixed, reflecting essentially that the number of oscillations of the radial electron distribution is gradually smaller; keep in mind that  $\eta - L = n - l$  is the degree of the Laguerre polynomials which controls the radial electron distribution. At the smaller dimension ( $d = 3$ ), a similar behavior is observed when  $l$  is fixed and  $n$  is increasing, while the opposite behavior occurs at the higher dimension ( $d = 12$ ). This indicates that the radial fluctuations are bigger in number as  $n$  increases and their amplitudes depend on the dimension  $d$  so that they are gradually smaller (bigger) at the high (small) dimension. This is because the dimension, hidden in both the hyperquantum numbers  $\eta$  and  $L$ , tunes the coefficients of the Laguerre polynomials and thus the amplitude height of the oscillations.

In the case of the Rényi quantity, which is a global spreading measure, the behavior for fixed  $l$  and  $n$  increasing is clearly increasing, whereas, for fixed  $n$ , it is slowly decreasing versus  $l$ ; this indicates that the radial electron distribution gradually spreads more and more (less and less) all over the

space when  $n(l)$  is increasing.

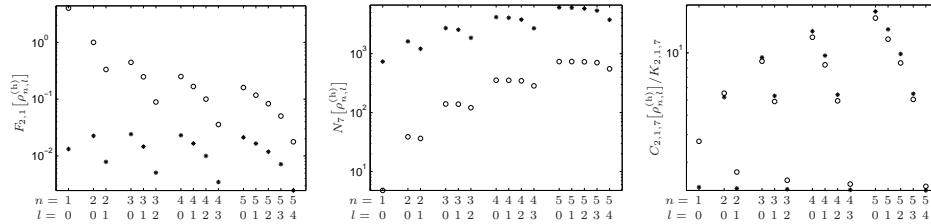


Figure 3: Fisher information  $F_{p,\beta}$  (left graph), Rényi entropy power  $N_\lambda$  (center graph), and  $(p, \beta, \lambda)$ -Fisher–Rényi complexity  $C_{p,\beta,\lambda}$  (right graph) of the radial hydrogenic distribution in position space with dimensions  $d = 3(\circ)$ ,  $12(*)$  versus the quantum numbers  $n$  and  $l$ . The complexity parameters are  $p = 2$ ,  $\beta = 1$ ,  $\lambda = 7$ .

Then, in Figure 4, the parameter dependence of the  $(p, \beta, \lambda)$ -Fisher–Rényi complexity  $C_{p,\beta,\lambda}$  (duly normalized to the lower bound) for the radial distribution of various states  $(n, l)$  of the  $d$ -dimensional hydrogenic system in position space with dimensions  $d = 3$  and  $12$ , is investigated for the sets  $(p, \beta, \lambda) = (2, .8, 7)$ ,  $(2, 1, 1)$  (usual Fisher–Shannon complexity) and  $(5, 2, 7)$ . Roughly speaking, the average behavior of the complexity versus  $(n, l)$  is similar for both dimensional cases to the one shown in the right graph of the previous figure. Of course, for a given pair  $(n, l)$ , the behavior of the complexity in terms of the dimension is quantitatively different according to the values of the parameters. Let us just point out, for instance, that the comparison of the behavior of  $C_{5,2,7}$  versus  $d$  and the corresponding ones of the other complexities shows that the complexity with higher value of  $p$  is more sensitive to the radial electron fluctuations with higher amplitudes.

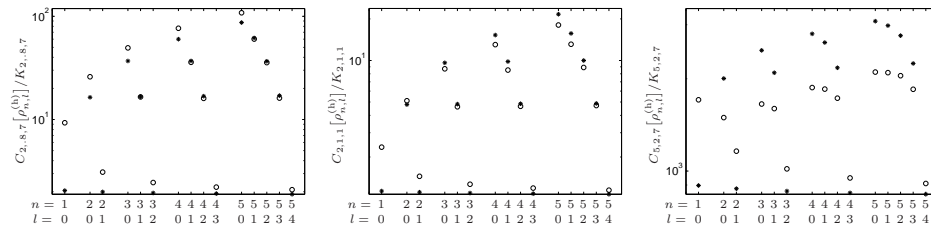


Figure 4:  $(p, \beta, \lambda)$ -Fisher–Rényi complexity (normalized to its lower bound),  $C_{p,\beta,\lambda}$ , with  $(p, \lambda, \beta) = (2, 0.8, 7)$ ,  $(2, 1, 1)$ ,  $(5, 2, 7)$  for the radial hydrogenic distribution in the position space with dimensions  $d = 3(\circ)$  and  $12(*)$ .

A similar study for the previous entropy- and complexity-like measures in momentum space has been done in Figures 5 and 6. Briefly, we observe that the behavior of these momentum quantities are in accordance with the analysis of the corresponding ones in position space, which has just been discussed. Note that here again the difference  $n - l$  determines the degree of the Gegenbauer polynomials that control the momentum density  $\gamma_{n,l}^{(h)}$ , so that the influence of  $n, l$  and  $d$  is formally similar to that for the position density  $\rho_{n,l}^{(h)}$ . Here, the influence of  $d$  on the height of the radial oscillation of the electron distribution (through the coefficients of the Gegenbauer polynomials) is the same for the two dimensionality cases considered in this work.

Let us highlight that the  $(n, l, d)$ -behavior of the Rényi power entropy in momentum space is just the opposite to the corresponding position one, manifesting the conjugacy of the two spaces, which is the spread of the position and momentum electron distributions are opposite.

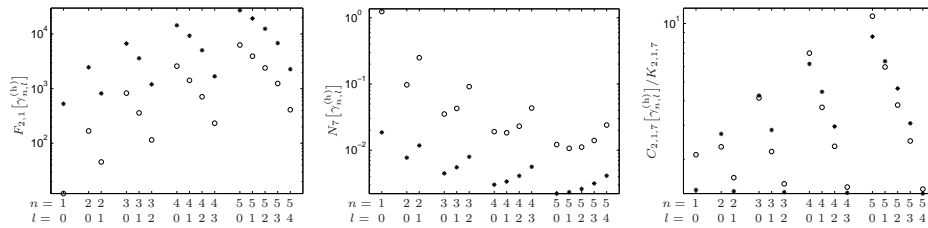


Figure 5: Fisher information  $F_{p,\beta}$  (left graph), Rényi entropy power  $N_\lambda$  (center graph), and  $(p, \beta, \lambda)$ -Fisher–Rényi complexity  $C_{p,\beta,\lambda}$  (right graph) of the radial hydrogenic distribution in momentum space with dimensions  $d = 3(\circ)$ ,  $12(*)$  versus the quantum numbers  $n$  and  $l$ . The complexity parameters are  $p = 2$ ,  $\beta = 1$ ,  $\lambda = 7$ .

### 4.3 $(p, \beta, \lambda)$ -Fisher–Rényi Complexity and the Harmonic System

The bound states of a  $d$ -dimensional harmonic (i.e., oscillator-like) system, where  $V(r) = \frac{1}{2}\omega^2 r^2$  (without loss of generality, the mass is assumed to be unity), are known to have the energies

$$E_n^{(o)} = \omega \left( 2n + L + \frac{3}{2} \right) \quad \text{with} \quad n = 0, 1, \dots, \quad l = 0, 1, \dots \quad (52)$$

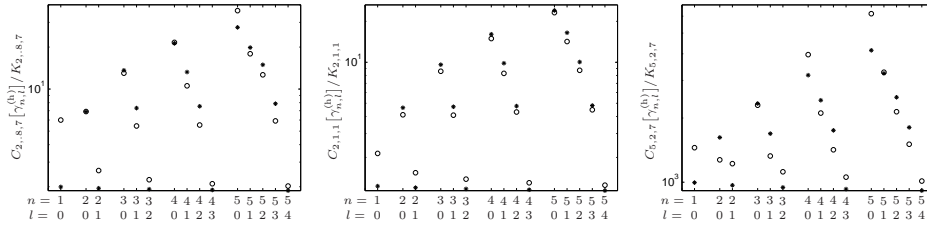


Figure 6:  $(p, \beta, \lambda)$ -Fisher–Rényi complexity (normalized to its lower bound),  $C_{p,\beta,\lambda}$ , with  $(p, \lambda, \beta) = (2, 0.8, 7)$ ,  $(2, 1, 1)$ ,  $(5, 2, 7)$  for the radial hydrogenic distribution in the momentum space with dimensions  $d = 3$ ( $\circ$ ) and  $12$ ( $*$ ).

(see e.g., [93, 94, 90]). The radial eigenfunctions writes in terms of the Laguerre polynomials as

$$\mathcal{R}_{n,l}^{(o)}(\tilde{r}) = \sqrt{R_{n,l}} \omega^{\frac{d-1}{4}} \tilde{r}^l e^{-\frac{1}{2}\tilde{r}^2} \mathcal{L}_n^{(L+\frac{1}{2})}(\tilde{r}^2), \tag{53}$$

where  $\tilde{r}$  is a dimensionless parameter, and the normalization coefficient  $R_{n,l}$  are given by

$$\tilde{r} = \sqrt{\omega} r \quad \text{and} \quad R_{n,l} = \frac{2\sqrt{\omega} \Gamma(n+1)}{\Gamma(n+L+\frac{3}{2})}, \tag{54}$$

respectively. Then, the associated radial position density is thus given by

$$\rho_{n,l}^{(o)}(r) = R_{n,l} \tilde{r}^{2L+2} e^{-\tilde{r}^2} \left[ \mathcal{L}_n^{(L+\frac{1}{2})}(\tilde{r}^2) \right]^2. \tag{55}$$

As for the hydrogenic system, using 8.971 in [87], one can compute  $\frac{d\rho_{n,l}^{(o)}}{dr} = \sqrt{\omega} \frac{d\rho_{n,l}^{(o)}}{d\tilde{r}}$ , and thus the  $(p, \beta, \lambda)$ -Fisher–Rényi of  $\rho_{n,l}^{(o)}$ . Remarkably,  $\mathcal{R}_{n,l}$  is invariant by the modified Hankel transform, so that the momentum radial density is formally the same as the position radial density.

For illustration purposes, we plot in Figure 7 the behavior of the Fisher information  $F_{2,1}$ , the Rényi entropy power  $N_7$  and the  $(2, 1, 7)$ -Fisher–Rényi complexity  $C_{2,1,7}$  of the radial position distribution of the  $d$ -dimensional harmonic system for various values of the quantum numbers  $n$  and  $l$  at the dimensions  $d = 3$  and  $12$ . Figure 8 depicts  $C_{p,\beta,\lambda}$  duly renormalized by its lower bound, for the triplets of complexity parameters  $(p, \beta, \lambda) = (2, .8, 7)$ ,  $(2, 1, 1)$  and  $(5, 2, 7)$ , respectively. In these graphs, one can make a similar interpretation as for the hydrogenic case. Note, however, that here the degree of

the Laguerre polynomials involved in the distribution  $\rho_{n,l}^{(o)}$  only depends on  $n$ ; this fact makes more regular the behavior of the previous information-theoretical measures in the oscillator case than in the hydrogenic one. Concomitantly, as  $n$  increases, the spreading of the distribution also increases. Conversely, parameters  $l$  and  $d$  have a relatively small influence on both the smoothness of the oscillation and on the spreading (compared to that of  $n$ ). Thus, unsurprisingly, both the Fisher information and the Rényi entropy power are weakly influenced by  $l$  (especially at the higher dimension) and by  $d$ . The Fisher–Rényi complexity, which quantifies the combined oscillatory and spreading effects, exhibits a very regular increasing behavior in terms of  $n$ .

Most interesting is the parameter-dependence of the complexity. Indeed, we can play with the complexity parameter to stress different aspects of the oscillator density and thus to reveal differences between the quantum states of the system. For instance, as one can see in Figure 8, the usual Fisher–Rényi complexity is unable to quantify the difference between the states of a given  $n$  versus the orbital number  $l$  and the dimension  $d$  (especially when  $n \geq 1$ , whereas the systems are quite different). This holds even playing with  $\lambda$  or  $\beta$ , while increasing parameter  $p$  (right graph), these states are distinguishable. This graph clearly shows the potentiality of the family of complexities  $C_{p,\beta,\lambda}$  to analyze a system, especially thanks to the full degree of freedom we have between the complexity parameters  $p$ ,  $\beta$  and  $\lambda$ .

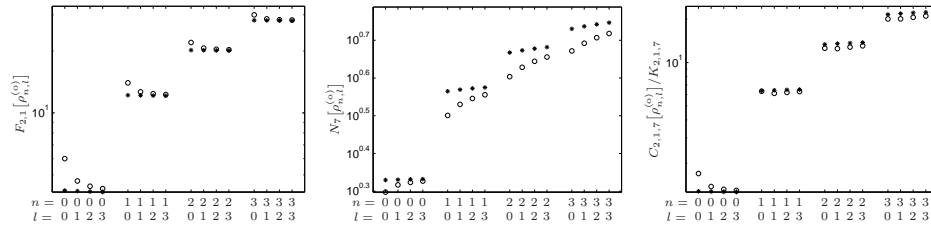


Figure 7: Fisher information  $F_{p,\beta}$  (left graph), Rényi entropy power  $N_\lambda$  (center graph), and  $(p, \beta, \lambda)$ -Fisher–Rényi complexity  $C_{p,\beta,\lambda}$  (right graph) versus  $n$  and  $l$  for the radial harmonic system in position space with dimensions  $d = 3(\circ)$ ,  $12(*)$ . The informational parameters are  $p = 2$ ,  $\beta = 1$ ,  $\lambda = 7$ .

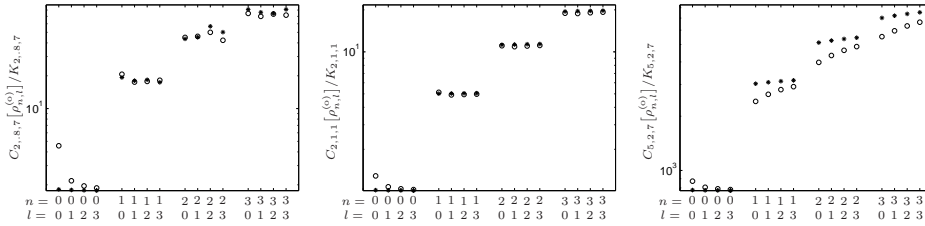


Figure 8:  $(p, \beta, \lambda)$ -Fisher–Rényi complexity (normalized to its lower bound)  $C_{p,\beta,\lambda}$  with  $(p, \lambda, \beta) = (2, 0.8, 7), (2, 1, 1), (5, 2, 7)$  for the oscillator system in the position space with dimensions  $d = 3(\circ), 12(*)$ .

## 5 Conclusions

In this paper, we have defined a three-parametric complexity measure of Fisher–Rényi type for a univariate probability density  $\rho$  that generalizes all the previously published quantifiers of the combined balance of the spreading and oscillatory facets of  $\rho$ . We have shown that this measure satisfies the three fundamental properties of a statistical complexity, namely, the invariance under translation and scaling transformations and the universal bounding from below. Moreover, the minimizing distributions are found to be closely related to the stretched Gaussian distributions. We have used an approach based on the Gagliardo–Nirenberg inequality and the differential-escort transformation of  $\rho$ . In fact, this inequality was previously used by Bercher and Lutwak et al. to find a biparametric extension of the celebrated Stam inequality which lowerbounds the product of the Rényi entropy power and the Fisher information. We have extended this biparametric Stam inequality to a three-parametric one by using the idea of differential-escort deformation of a probability density.

Then, we have numerically analyzed the previous entropy-like quantities and the three-parametric complexity measure for various specific quantum states of the two main prototypes of multidimensional electronic systems subject to a central potential of Coulomb (the  $d$ -dimensional hydrogenic atom) and harmonic (the  $d$ -dimensional isotropic harmonic oscillator) character. Briefly, we have found that the proposed complexity allows to capture and quantify the delicate balance of the gradient and the spreading contents of the radial electron distribution of ground and excited states of the system. The variation of the three parameters of the proposed complexity allows one to stress differently this balance in the various radial regions of the charge distribution.

The results found in this work can be generalized in various ways that remain open. Indeed, the Gagliardo–Nirenberg relation is quite powerful since it involves the  $p$ -norm of the function  $u$ , the  $q$ -norm of its  $j$ -th derivative and the  $s$ -norm of its  $m$ -th derivative, where  $p, q, s$  and the integers  $j, m$  are linked by inequalities (see [95]). This leaves open the possibility to define still more extended (complete) complexity measures, with higher-order (in terms of derivative) measures of information. Even more interesting, this inequality-based relation holds for any dimension  $d \geq 1$ ; thus, it supports the possibility to extend our univariate results to multidimensional distributions, but with tighter restrictions on the parameters. The main difficulty in this case is related with the multidimensional extension of the validity domain by using the differential-escort technique or a similar one.

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**authorcontributions**The authors contributed equally to this work.

## A Proof of Proposition 2

### A.1 The Case $\lambda \neq 1$

The result of the proposition is a direct consequence of the Gagliardo–Nirenberg inequality [95, 52, 35], stated in our context as follows: let  $p > 1$ ,  $s > q \geq 1$  and  $\theta = \frac{p(s-q)}{s(p+pq-q)}$ ; then, there exists an optimal strictly positive constant  $K$ , depending only on  $p, q$  and  $s$  such that for any function  $u : \mathbb{R} \mapsto \mathbb{R}_+$ ,

$$K \left\| \frac{d}{dx} u \right\|_p^\theta \|u\|_q^{1-\theta} \geq \|u\|_s, \quad (56)$$

provided that the involved quantities exist, the equality being achieved for  $u$  solution of the differential equation

$$-\frac{d}{dx} \left( \left| \frac{d}{dx} u \right|^{p-2} \frac{d}{dx} u \right) + u^{q-1} = \gamma u^{s-1}, \quad (57)$$



where  $\gamma > 0$  is such that  $\|u\|_s$  is fixed and can be chosen arbitrarily (it corresponds to a Lagrange multiplier, see Equations (26) and (27) in [52]). Finding  $u$  thus allows to determine the optimal constant  $K$ . Note that, if the equality in 56 is reached for  $u_\gamma$ , then it is also reached for  $\bar{u}_\gamma = \delta u_\gamma(x)$  for any  $\delta > 0$ . One can see that  $\bar{u}_\gamma$  satisfies the differential equation  $-\frac{d}{dx} \left( \left| \frac{d}{dx} \bar{u} \right|^{p-2} \frac{d}{dx} \bar{u} \right) + \delta^{p-q} \bar{u}^{q-1} - \gamma \delta^{p-s} \bar{u}^{s-1} = 0$ . Thus, function  $u$  reaching the equality in Equation 56 can also be chosen as the solution of the differential equation  $-\frac{d}{dx} \left( \left| \frac{d}{dx} u \right|^{p-2} \frac{d}{dx} u \right) + \kappa u^{q-1} - \zeta u^{s-1} = 0$ , where  $\kappa > 0$  and  $\zeta > 0$  can be chosen arbitrarily. As we will see later on, a judicious choice allowing to include the limit case  $s \rightarrow q$  is to take  $\kappa = \zeta = \frac{\gamma}{s-q}$ , i.e., to chose function  $u$  reaching the equality in Equation 56 as the solution of the differential equation

$$-\frac{d}{dx} \left( \left| \frac{d}{dx} u \right|^{p-2} \frac{d}{dx} u \right) + \gamma \frac{u^{q-1} - u^{s-1}}{s - q} = 0, \tag{58}$$

where  $\gamma > 0$  can be arbitrarily chosen.

**A.1.1 The Sub-Case  $\lambda < 1$**

Following the very same steps than in [35], let us consider first

$$\lambda = \frac{q}{s} < 1.$$

With  $u^s$  integrable, one can normalize it, that is, writing it under the form  $u = \rho^{\frac{1}{s}} = \rho^{\frac{\lambda}{q}}$  with  $\rho$  a probability density function. Thus,  $\|u\|_s = 1$  and from the Gagliardo–Nirenberg inequality,

$$\left\| \rho^{\frac{\lambda}{q}-1} \frac{d}{dx} \rho \right\|_p^\theta \left\| \rho^{\frac{\lambda}{q}} \right\|_q^{1-\theta} \geq s^\theta K^{-1}.$$

Simple algebra allows to write the terms of the left-hand side in terms of the generalized Fisher information and of the Rényi entropy power, respectively, to conclude that

$$\left( F_{p, \frac{\lambda}{q} - \frac{1}{p} + 1}[\rho] \right)^{\frac{\theta}{p} \frac{p(\frac{\lambda}{q} - \frac{1}{p} + 1)}{2}} \left( N_\lambda[\rho] \right)^{\frac{1-\theta}{q} \frac{1-\lambda}{2}} \geq s^\theta K^{-1}. \tag{59}$$

Using  $1 - \frac{1}{p} = \frac{1}{p^*}$ , let us then denote

$$\beta = \frac{\lambda}{q} + \frac{1}{p^*} = \frac{1}{s} + \frac{1}{p^*},$$

and note that the conditions imposed on  $p, q$  and  $s$  together with  $\lambda > 0$  impose

$$\beta \in \left( \frac{1}{p^*}; \frac{1}{p^*} + \lambda \right],$$

once  $p$  and  $\lambda$  are given. Simple algebra allows thus to show that  $\frac{\theta}{p} \frac{p \left( \frac{\lambda + \frac{1}{p^*}}{2} \right)}{2} = \frac{1-\theta}{q} \frac{1-\lambda}{2} = \frac{\theta\beta}{2} > 0$ : the exponent of the Fisher information and of the entropy power in Equation 59 are thus equal. Moreover,  $\theta$  being strictly positive, both sides of Equation 59 can be elevated to exponent  $\frac{2}{\theta}$  leading to the result of the proposition, where the bound is given by

$$K_{p,\beta,\lambda} = s^2 K^{-\frac{2}{\theta}}, \tag{60}$$

where  $s$  and  $\theta$  can be expressed by their parametrization in  $p, \beta, \lambda$ . Finally, the differential equation 10 satisfied by the minimizer  $u$  comes from Equation 58 noting that  $s = \frac{p^*}{\beta p^* - 1}$  and  $q = \frac{\lambda p^*}{\beta p^* - 1}$ , remembering that  $\rho = u^s$  and thus that  $\gamma$  is to be chosen such that  $u^s$  sums to unity.

**A.1.2 The Sub-Case  $\lambda > 1$**

Consider now

$$\lambda = \frac{s}{q} > 1$$

and  $u = \rho^{\frac{1}{q}} = \rho^{\frac{\lambda}{s}}$ , leading to

$$\left( F_{p, \frac{\lambda}{s} - \frac{1}{p} + 1}[\rho] \right)^{\frac{\theta}{p} \frac{p \left( \frac{\lambda}{s} - \frac{1}{p} + 1 \right)}{2}} \left( N_\lambda[\rho] \right)^{-\frac{1}{s} \frac{1-\lambda}{2}} \geq q^\theta K^{-1}. \tag{61}$$

Denoting now

$$\beta = \frac{\lambda}{s} + \frac{1}{p^*} = \frac{1}{q} + \frac{1}{p^*},$$

imposing

$$\beta \in \left( \frac{1}{p^*}; \frac{1}{p^*} + 1 \right]$$

once  $p$  and  $\lambda$  are given. Simple algebras allows thus to show that  $\frac{\theta}{p} \frac{p \left( \frac{\lambda}{s} - \frac{1}{p} + 1 \right)}{2} = -\frac{1}{s} \frac{1-\lambda}{2} = \frac{\theta\beta}{2} > 0$ : again, the exponent of the Fisher information and of the entropy power in Equation 61 are equal. Here again,  $\theta > 0$  allowing to elevate both side of Equation 61 to exponent  $\frac{2}{\theta}$ . The bound is now given by

$$K_{p,\beta,\lambda} = q^2 K^{-\frac{2}{\theta}} \tag{62}$$

where  $q$  and  $\theta$  can be expressed by their parametrization in  $p, \beta, \lambda$ . Finally, as for the previous case, the differential equation 10 satisfied by the minimizer  $u$  comes from Equation 58 noting that now  $q = \frac{p^*}{\beta p^* - 1}$  and  $s = \frac{\lambda p^*}{\beta p^* - 1}$ , remembering that now  $\rho = u^q$  and thus that  $\gamma$  is to be chosen such that  $u^q$  sums to unity.

### A.2 The Case $\lambda = 1$

The minimizer for  $\lambda = 1$  can be viewed as the limiting case  $\lambda \rightarrow 1$ , i.e.,  $s \rightarrow q$ .

One can also proceed as done by Agueh in [52] to determine the sharp bound of the Gagliardo–Nirenberg inequality. To this end, let us consider the minimization problem

$$\inf \left\{ \frac{1}{p} \int_{\mathbb{R}} \left| \frac{d}{dx} u(x) \right|^p dx - \frac{1}{q} \int_{\mathbb{R}} [u(x)]^q \log u(x) dx : u \geq 0, \int_{\mathbb{R}} [u(x)]^q dx = 1 \right\} \quad (63)$$

for  $p > 1$  and  $q \geq 1$  (see Chapters 5 and 6 in [96, ] justifying the existence of a minimum). Hence, there exists an optimal constant  $K$  such that for any function  $u$  such that  $u^q$  sums to unity,

$$\frac{1}{p} \int_{\mathbb{R}} \left| \frac{d}{dx} u(x) \right|^p dx - \frac{1}{q} \int_{\mathbb{R}} [u(x)]^q \log u(x) dx \geq K. \quad (64)$$

Now, fix a function  $u$  and consider  $v(x) = \gamma^{\frac{1}{q}} u(\gamma x)$  for some  $\gamma > 0$ .  $v^q$  also sums to unity and thus can be put in the previous inequality, leading to

$$f_u(\gamma) \equiv \frac{\gamma^{\frac{p}{q} + p - 1}}{p} \int_{\mathbb{R}} \left| \frac{d}{dx} u(x) \right|^p dx - \frac{1}{q} \int_{\mathbb{R}} [u(x)]^q \log u(x) dx - \frac{1}{q^2} \log \gamma \geq K \quad (65)$$

for any  $\gamma > 0$ . Thus, this inequality is necessarily satisfied for the  $\gamma$  that minimizes  $f_u(\gamma)$ . A rapid study of  $f_u$  allows to conclude that it is minimum for

$$\gamma = \left( \frac{p}{q(p + q(p - 1)) \int_{\mathbb{R}} \left| \frac{d}{dx} u(x) \right|^p dx} \right)^{\frac{q}{p + q(p - 1)}}. \quad (66)$$

Now, injecting Equation 66 in Equation 65 gives

$$\frac{1}{p + q(p - 1)} \log \int_{\mathbb{R}} \left| \frac{d}{dx} u(x) \right|^p dx - \int_{\mathbb{R}} [u(x)]^q \log u(x) dx \geq \tilde{K}, \quad (67)$$

with  $\tilde{K} = qK + \frac{1}{p+q(p-1)} \left( \log \left( \frac{p}{q(p+q(p-1))} \right) - 1 \right)$ . Consider now  $u_{\min}$  the minimizer of problem 63. Obviously,  $f_{u_{\min}}(\gamma)$  is minimum for  $\gamma = 1$ , that gives, from Equation 66,  $\int_{\mathbb{R}} \left| \frac{d}{dx} u_{\min}(x) \right|^p dx = \frac{p}{q(p+q(p-1))}$  and from Equation 64, being an equality,  $\int_{\mathbb{R}} [u_{\min}(x)]^q \log u_{\min}(x) dx = \frac{1}{p+q(p-1)} - qK$ . Injecting these expressions in Equation 67 allows concluding that this inequality is sharp, and moreover that its minimizer coincides with that of the minimization problem 63.

Inequality 8 is obtained by injecting  $u = \rho^{\frac{1}{q}}$  in Equation 67 and after some trivial algebra and denoting  $\beta = \frac{1}{q} + \frac{1}{p^*} \in \left( \frac{1}{p^*}; 1 + \frac{1}{p^*} \right]$ , confirming that it can be viewed as a limit case  $\lambda \rightarrow 1$ .

Let us now solve the minimization problem 63, that is, from the Lagrangian technique [97], to minimize  $\int_{\mathbb{R}} F(x, u, u') dx$ , where  $F(x, u, u') = \frac{1}{p} \left| \frac{d}{dx} u(x) \right|^p - \frac{1}{q} [u(x)]^q \log u(x) - \gamma [u(x)]^q$  and where  $u' = \frac{d}{dx} u$  and  $\gamma$  is the Lagrange multiplier. The solution of this variational problem is given by the Euler–Lagrange equation [97],  $\frac{\partial F}{\partial u} - \frac{d}{dx} \left( \frac{\partial F}{\partial u'} \right) = 0$ , that writes here after a re-parametrization  $\delta = \frac{1}{q} + q\gamma$

$$-\frac{d}{dx} \left( \left| \frac{d}{dx} u \right|^{p-2} \frac{d}{dx} u \right) - u^{q-1} (\log u + \delta) = 0. \tag{68}$$

$\delta$  is to be determined a posteriori so as to satisfy the constraint  $\int_{\mathbb{R}} [u(x)]^q dx = 1$ . Again, one can easily see that if the bound in Equation 67 is achieved for  $u_{\min}$ , then it is also achieved for  $\bar{u}_{\delta}(x) = \sigma u_{\min}(\sigma^q x)$  whatever  $\sigma > 0$ . Reporting  $u_{\min}(x) = \sigma^{-1} \bar{u}_{\sigma}(\sigma^{-q} x)$  in the differential equation allows to see that  $\bar{u}_{\sigma}$  is a solution of the differential equation  $-\frac{d}{dx} \left( \left| \frac{d}{dx} \bar{u} \right|^{p-2} \frac{d}{dx} \bar{u} \right) - \sigma^{p+q(p-1)} \bar{u}^{q-1} (\log \bar{u} - \log \sigma + \delta) = 0$ . Choosing  $\sigma = \exp(\delta)$  and rewriting  $\sigma^{p+q(p-1)} = \gamma$ , one can thus choose the minimizer  $u$  as the solution of the differential equation

$$-\frac{d}{dx} \left( \left| \frac{d}{dx} u \right|^{p-2} \frac{d}{dx} u \right) - \gamma u^{q-1} \log u = 0, \tag{69}$$

where  $\gamma$  is to be determined a posteriori so as to satisfy the constraint  $\int_{\mathbb{R}} [u(x)]^q dx = 1$ . This result is precisely the limit case of the differential equation 58 when  $s \rightarrow q$ .

## B Proof of Proposition 3

For  $\lambda = 1$ , Relations 12 and 13 induced by Transform 11 of the indexes are obvious since  $\mathfrak{T}_p(\beta, 1) = (\beta, 1)$ .

Then, for  $\lambda \neq 1$ , Relation 12 comes from the fact that the function  $u$  solution of Equation 58 depends only on  $p, q$  and  $s$ . Let us write  $(\beta, \lambda)$  and  $\vartheta$  the parameters for the first situation of the above proof, i.e.,  $\lambda = \frac{q}{s}$  and  $\beta = \frac{1}{s} + \frac{1}{p^*} = \frac{\lambda}{q} + \frac{1}{p^*}$ , and  $(\bar{\beta}, \bar{\lambda})$  and  $\bar{\vartheta}$  the parameters for the second situation, i.e.,  $\bar{\lambda} = \frac{s}{q}$  and  $\bar{\beta} = \frac{1}{q} + \frac{1}{p^*} = \frac{\bar{\lambda}}{s} + \frac{1}{p^*}$ . It is straightforward to see that  $\bar{\lambda} = \frac{1}{\lambda}$  and  $\bar{\beta} = \frac{\beta}{\lambda} - \frac{1}{\lambda p^*} + \frac{1}{p^*} = \frac{\beta p^* + \lambda - 1}{\lambda p^*}$ , i.e.,  $(p, \bar{\beta}, \bar{\lambda}) = (p, \mathfrak{T}_p(\beta, \lambda))$ , and, conversely, that  $(p, \beta, \lambda) = (p, \mathfrak{T}_p(\bar{\beta}, \bar{\lambda}))$ . Since the optimal  $u$  is fixed once  $p, q$  and  $s$  are given, one has  $u_{p, \mathfrak{T}_p(\beta, \lambda)} = u_{p, \beta, \lambda}$ . Finally, simple algebra allows to show that  $\bar{\vartheta} = \lambda \vartheta$  and  $\vartheta = \bar{\lambda} \bar{\vartheta}$ , which finishes the proof.

Now, Relation 13 immediately comes from Equations 60 and 62 together with  $\lambda = \frac{q}{s}$ .

## C Proof of Proposition 5

### C.1 The $(p, \beta, \lambda)$ -Fisher–Rényi Complexity is Lowerbounded over $\tilde{\mathcal{D}}_p$

As detailed in the text, consider a point  $(\beta, \lambda) \in \tilde{\mathcal{D}}_p$ . Thus, there exists an index  $\alpha > 0$  such that  $\mathfrak{A}_\alpha(\beta, \lambda) \in \mathcal{L}_p \cup \bar{\mathcal{L}}_p$ . Applying Propositions 2 and 4, we have

$$\begin{aligned} C_{p, \beta, \lambda}[\rho] &= \alpha^2 C_{p, \mathfrak{A}_\alpha(\beta, \lambda)}[\mathfrak{E}_\alpha[\mathfrak{E}_{\alpha^{-1}}[\rho]]] \\ &\geq \alpha^2 K_{p, \mathfrak{A}_\alpha(\beta, \lambda)} \equiv K_{p, \beta, \lambda}. \end{aligned}$$

Finally, denoting  $(\tilde{\beta}, \tilde{\lambda}) = \mathfrak{A}_\alpha(\beta, \lambda)$ , the minimizers satisfy  $\mathfrak{E}_{\alpha^{-1}}[\rho_{p, \beta, \lambda}] = g_{p, \tilde{\lambda}}$  (see Section 2.3.1), or  $\mathfrak{E}_{\alpha^{-1}}[\rho_{p, \beta, \lambda}] = g_{p, 2-\tilde{\lambda}}$  (see Section 2.3.2), that is,

$$\rho_{p, \beta, \lambda} = \begin{cases} \mathfrak{E}_\alpha[g_{p, \tilde{\lambda}}], & \text{if } \mathfrak{A}_\alpha(\beta, \lambda) \in \mathcal{L}_p, \\ \mathfrak{E}_\alpha[g_{p, 2-\tilde{\lambda}}], & \text{if } \mathfrak{A}_\alpha(\beta, \lambda) \in \bar{\mathcal{L}}_p. \end{cases}$$

### C.2 Explicit Expression for the Minimizers.

In the sequel, we determine the differential-escort transformation  $\mathfrak{E}_\alpha[g_{p,\lambda}]$  with  $\lambda < 1$ . Let us denote by  $Z_{p,\lambda} = \int_{\mathbb{R}} \left(1 + (1 - \lambda)|x|^{p^*}\right)^{\frac{1}{\lambda-1}} dx = \frac{2 B\left(\frac{1}{p^*}, \frac{1}{1-\lambda} - \frac{1}{p^*}\right)}{p^*(1-\lambda)^{\frac{1}{p^*}}}$  the normalization coefficient of the distribution  $g_{p,\lambda}$  [35, 87]). Hence, as defined in Definition (5),  $\mathfrak{E}_\alpha[g_{p,\lambda}](y) = \left[g_{p,\lambda}(x(y))\right]^\alpha$  with

$$\begin{aligned} \frac{dy}{dx} &= \left[g_{p,\lambda}(x)\right]^{1-\alpha} \\ &= Z_{p,\lambda}^{\alpha-1} \left(1 + (1 - \lambda)|x|^{p^*}\right)^{\frac{1-\alpha}{\lambda-1}}. \end{aligned}$$

Thus,  $y(x)$  writes

$$\begin{aligned} y(x) &= Z_{p,\lambda}^{\alpha-1} \operatorname{sign}(x) \int_0^{|x|} \left(1 + (1 - \lambda)t^{p^*}\right)^{\frac{1-\alpha}{\lambda-1}} dt \\ &= \kappa_{p,\lambda,\alpha} \operatorname{sign}(x) \int_0^{\frac{(1-\lambda)|x|^{p^*}}{1+(1-\lambda)|x|^{p^*}}} \tau^{\frac{1}{p^*}-1} (1 - \tau)^{\frac{\alpha-1}{\lambda-1} - \frac{1}{p^*}-1} d\tau \end{aligned}$$

when making the change of variables  $\tau = \frac{(1-\lambda)t^{p^*}}{1+(1-\lambda)t^{p^*}}$  and denoting  $\kappa_{p,\lambda,\alpha} = \frac{Z_{p,\lambda}^{\alpha-1}}{p^*(1-\lambda)^{\frac{1}{p^*}}}$ . One can recognize in the integral the incomplete beta function  $\mathfrak{B}(a, b, x) = \int_0^x t^{a-1}(1-t)^{b-1} dt$  defined when  $\Re\{a\} > 0$  and for  $x \in [0; 1)$  [85]. Here,  $a = \frac{1}{p^*} > 0$ ,  $b = \frac{\alpha-1}{\lambda-1} - \frac{1}{p^*}$  and noting that  $\frac{(1-\lambda)|x|^{p^*}}{1+(1-\lambda)|x|^{p^*}} \in [0; 1)$ . Hence,

$$y(x) = \kappa_{p,\lambda,\alpha} \operatorname{sign}(x) \mathfrak{B}\left(\frac{1}{p^*}, \frac{\alpha-1}{\lambda-1} - \frac{1}{p^*}; \frac{(1-\lambda)|x|^{p^*}}{1+(1-\lambda)|x|^{p^*}}\right). \quad (70)$$

Note that  $\frac{y}{\kappa_{p,\lambda,\alpha}} : \mathbb{R} \mapsto \left(-B\left(\frac{1}{p^*}, \frac{\alpha-1}{\lambda-1} - \frac{1}{p^*}\right); B\left(\frac{1}{p^*}, \frac{\alpha-1}{\lambda-1} - \frac{1}{p^*}\right)\right)$ , where  $B(a, b) = \lim_{x \rightarrow 1} \mathfrak{B}(a, b, x)$  is the beta function [85, 87, 86];  $B(a, b)$  is thus infinite when  $b \leq 0$ .

Denoting  $\mathfrak{B}^{-1}$  the inverse of incomplete beta function, we obtain

$$1 + (1 - \lambda)|x(y)|^{p^*} = \frac{1}{1 - \mathfrak{B}^{-1}\left(\frac{1}{p^*}, \frac{\alpha-1}{\lambda-1} - \frac{1}{p^*}; \frac{|y|}{\kappa_{p,\lambda,\alpha}}\right)} \quad (71)$$

and, thus,

$$\mathfrak{E}_\alpha [g_{p,\lambda}] (y) \propto \left[ 1 - \mathfrak{B}^{-1} \left( \frac{1}{p^*}, \frac{\alpha - 1}{\lambda - 1} - \frac{1}{p^*}; \frac{|y|}{\kappa_{p,\lambda,\alpha}} \right) \right]^{\frac{\alpha}{1-\lambda}} \mathbb{1}_{\left[0; B\left(\frac{1}{p^*}, \frac{\alpha-1}{\lambda-1} - \frac{1}{p^*}\right)\right]} \left( \frac{|y|}{\kappa_{p,\lambda,\alpha}} \right) \quad (72)$$

Note that from  $\mathfrak{B}(a, -a, x) = a^{-1} \left( \frac{x}{1-x} \right)^a$  [87, 86]), we naturally recover that  $\mathfrak{E}_1 [g_{p,\lambda}] = g_{p,\lambda}$ .

Finally, let us remark that

$$\tilde{\mathcal{D}}_p = \{(\beta, \lambda) \in \mathbb{R}_+^{*2} : 1 - p^* \beta < \lambda < 1\} \cup \{(\beta, \lambda) \in \mathbb{R}_+^{*2} : \lambda > 1\} \cup \{(\beta, 1), \beta \in \mathbb{R}_+^*\}, \quad (73)$$

the first ensemble being a subset of  $\mathfrak{A}[\mathcal{L}_p]$  and the second one a subset of  $\mathfrak{A}[\bar{\mathcal{L}}_p]$ . We treat now these three cases separately.

### C.2.1 The Case $1 - p^* \beta < \lambda < 1$

Following Appendix C.1, let us first determine  $\alpha$  such that  $\mathfrak{A}_\alpha(\beta, \lambda) \in \mathcal{L}_p$ , which is  $\alpha$  such that  $\alpha\beta = 1 + \alpha(\lambda - 1)$ . Hence,

$$\alpha = \frac{1}{\beta + 1 - \lambda} \quad \text{and} \quad \mathfrak{A}_\alpha(\beta, \lambda) = \left( \frac{\beta}{\beta + 1 - \lambda}, \frac{\beta}{\beta + 1 - \lambda} \right). \quad (74)$$

The fact that  $\beta > 0$  and  $\lambda < 1$  insures that  $\beta + 1 - \lambda \neq 0$ .

From Sections 2.3.1 and C.1, the minimizer of the complexity is thus given by

$$\rho_{p,\beta,\lambda} = \mathfrak{E}_{\frac{1}{\beta+1-\lambda}} \left[ g_{p, \frac{\beta}{\beta+1-\lambda}} \right]. \quad (75)$$

One can easily see that  $\frac{\beta}{\beta+1-\lambda} \in \left( \frac{1}{1+p^*}; 1 \right)$ , and thus we immediately get from Equation 72,

$$\rho_{p,\beta,\lambda}(x) \propto \left[ 1 - \mathfrak{B}^{-1} \left( \frac{1}{p^*}, \frac{\beta - \lambda}{1 - \lambda} - \frac{1}{p^*}; \frac{|y|}{\kappa_{p,\alpha\beta,\alpha}} \right) \right]^{\frac{1}{1-\lambda}} \mathbb{1}_{\left[0; B\left(\frac{1}{p^*}, \frac{\beta-\lambda}{1-\lambda} - \frac{1}{p^*}\right)\right]} \left( \frac{|y|}{\kappa_{p,\alpha\beta,\alpha}} \right). \quad (76)$$

Noting that  $\frac{\beta-\lambda}{1-\lambda} = \frac{\beta-1}{1-\lambda} + \frac{1}{p}$ , it appears that this density is nothing more than the  $(p, \beta, \lambda)$ -Gaussian of Definition 6 (remember that the families of density are defined up to a shift and a scaling).

**C.2.2 The Case  $\lambda > 1$**

Following again Appendix C.1, let us first determine  $\alpha$  such that  $\mathfrak{A}_\alpha(\beta, \lambda) \in \overline{\mathcal{L}}_p$ , i.e., such that  $\alpha\beta = \frac{p^*+1-[1+\alpha(\lambda-1)]}{p^*}$ . We thus obtain

$$\alpha = \frac{p^*}{p^*\beta + \lambda - 1} \quad \text{and} \quad \mathfrak{A}_\alpha(\beta, \lambda) = \left( \frac{p^*\beta}{p^*\beta + \lambda - 1}, 1 + \frac{p^*(\lambda - 1)}{p^*\beta + \lambda - 1} \right). \tag{77}$$

The fact that  $\beta > 0$  and  $\lambda > 1$  insures that  $p^*\beta + \lambda - 1 \neq 0$ .

From Section 2.3.1 and Appendix C.1, the minimizers for the complexity expresses

$$\rho_{p,\beta,\lambda} = \mathfrak{E}_{\frac{p^*}{p^*\beta + \lambda - 1}} \left[ g_{p,1-\frac{p^*(\lambda-1)}{p^*\beta + \lambda - 1}} \right]. \tag{78}$$

One can easily has that  $1 - \frac{p^*(\lambda-1)}{p^*\beta + \lambda - 1} \in (1 - p^*; 1)$  and thus we immediately get from Equation 72

$$\rho_{p,\beta,\lambda}(y) \propto \left[ 1 - \mathfrak{B}^{-1} \left( \frac{1}{p^*}, \frac{\beta - 1}{\lambda - 1}; \frac{|y|}{\kappa_{p,1-\alpha(\lambda-1),\alpha}} \right) \right]^{\frac{1}{\lambda-1}} \mathbb{1}_{[0; B(\frac{1}{p^*}, \frac{\beta-1}{\lambda-1})]} \left( \frac{|y|}{\kappa_{p,1-\alpha(\lambda-1),\alpha}} \right). \tag{79}$$

The density is again nothing more than the  $(p, \beta, \lambda)$ -Gaussian of Definition 6.

**C.2.3 The Case  $\lambda = 1$**

We exclude here the trivial point  $\beta = 1$ . Now, taking  $\alpha = \frac{1}{\beta}$  gives  $\mathfrak{A}_\alpha(\beta, 1) = (1, 1)$ .

We know that the minimizer for  $\beta = 1$  is given by  $g_{p,1}(x) = Z_{p,1}^{-1} \exp(-|x|^{p^*})$  with

$$Z_{p,1} = \int_{\mathbb{R}} \exp(-|x|^{p^*}) dx = \frac{2\Gamma\left(\frac{1}{p^*}\right)}{p^*} \quad [35, 87].$$

Following again Appendix C.1, we have to determine

$$\mathfrak{E}_{\frac{1}{\beta}} \left[ g_{p,1} \right](y) = [g_{p,1}(x(y))]^{\frac{1}{\beta}} = Z_{p,1}^{-\frac{1}{\beta}} \exp\left(-\frac{|x(y)|^{p^*}}{\beta}\right) \tag{80}$$

with

$$\begin{aligned} \frac{dy}{dx} &= [g_{p,1}]^{1-\frac{1}{\beta}} \\ &= Z_{p,1}^{\frac{1-\beta}{\beta}} \exp\left(-\frac{\beta-1}{\beta}|x|^{p^*}\right), \end{aligned}$$



and thus

$$y(x) = Z_{p,1}^{\frac{1-\beta}{\beta}} \text{sign}(x) \int_0^{|x|} \exp\left(-\frac{\beta-1}{\beta} t^{p^*}\right) dt.$$

Viewing this integral in the complex plane (here in the real line), one can make the change of variables  $\tau = \frac{\beta-1}{\beta} t^{p^*}$ , i.e.,  $t = \left(\frac{\beta-1}{\beta}\right)^{-\frac{1}{p^*}} \tau^{\frac{1}{p^*}}$  to obtain

$$y(x) = \frac{Z_{p,1}^{\frac{1-\beta}{\beta}}}{p^* \left(\frac{\beta-1}{\beta}\right)^{\frac{1}{p^*}}} \text{sign}(x) \int_0^{\frac{\beta-1}{\beta} |x|^{p^*}} \tau^{\frac{1}{p^*}-1} \exp(-\tau) d\tau, \quad (81)$$

where  $\left(\frac{\beta-1}{\beta}\right)^{\frac{1}{p^*}}$  is complex in general, real only if  $\frac{\beta-1}{\beta} \geq 0$ , i.e., if  $\beta \notin (0; 1)$ . One can recognize in the integral the incomplete gamma function  $\mathfrak{G}(a, x) = \int_0^x t^{a-1} \exp(-t) dt$ , defined for  $\Re\{a\} > 0$  and for any complex  $x$  [85]. We then obtain,

$$y(x) = \kappa_{p,\beta} \text{sign}(x) \left[ \left(\frac{\beta-1}{\beta}\right)^{-\frac{1}{p^*}} \mathfrak{G}\left(\frac{1}{p^*}; \frac{\beta-1}{\beta} |x|^{p^*}\right) \right], \quad (82)$$

where  $\kappa_{p,\beta} = \frac{Z_{p,1}^{\frac{1-\beta}{\beta}}}{p^*}$ . Note that the term in square brackets is real and positive, and takes its values over  $\mathbb{R}_+$  if  $\beta > 1$  (remember that we excluded the trivial situation  $\beta = 1$ ), and over  $\left[0; \Gamma\left(\frac{1}{p^*}\right)\right)$  if  $\beta < 1$ .

Denoting  $\mathfrak{G}^{-1}$  the inverse of the incomplete gamma function, this gives

$$\frac{1}{\beta} |x(y)|^p = \frac{1}{\beta-1} \mathfrak{G}^{-1}\left(\frac{1}{p^*}; \left(\frac{\beta-1}{\beta}\right)^{\frac{1}{p^*}} \frac{|y|}{\kappa_{p,1}}\right) \quad (83)$$

defined for  $\frac{|y|}{\kappa_{p,1}} < \frac{\Gamma(1/p^*)}{\mathbb{1}_{(0;1)}(\beta)}$  with the convention  $1/0 = +\infty$ . We thus achieve

$$\rho_{p,\beta,1}(y) \propto \exp\left(\frac{1}{1-\beta} \mathfrak{G}^{-1}\left(\frac{1}{p^*}; \left(\frac{\beta-1}{\beta}\right)^{\frac{1}{p^*}} \frac{|y|}{\kappa_{p,1}}\right)\right) \mathbb{1}_{\left[0; \frac{\Gamma(1/p^*)}{\mathbb{1}_{(0;1)}(\beta)}\right)}\left(\frac{|y|}{\kappa_{p,1}}\right). \quad (84)$$

We again recover the  $(p, \beta, \lambda)$ -Gaussian.

### C.3 Symmetry through the Involution $\mathfrak{T}_p$ .

For  $\lambda = 1$ , the result is trivial since  $\mathfrak{T}_p(\beta, 1) = (\beta, 1)$  (see Equation 11).

Now, for  $\lambda \neq 1$ , let us denote  $(\bar{\beta}, \bar{\lambda}) = \mathfrak{T}_p(\beta, \lambda) = \left(\frac{p^*\beta + \lambda - 1}{p^*\lambda}, \frac{1}{\lambda}\right)$  the involutory transform of  $(\beta, \lambda)$ . Some simple algebra allows to show that if  $1 - \beta p^* < \lambda < 1$ , then  $\bar{\lambda} > 1$ , and reciprocally. Thus, it is straightforward to see that  $q_{p, \mathfrak{T}_p(\beta, \lambda)} = q_{p, \beta, \lambda}$  and that  $\frac{1}{|\bar{1} - \bar{\lambda}|} = \frac{\lambda}{|1 - \lambda|}$ , leading to

$$g_{p, \mathfrak{T}_p(\beta, \lambda)} \propto \left[ g_{p, \beta, \lambda} \right]^\lambda. \tag{85}$$

Now, if  $\lambda < 1$ , the optimal bound is given by  $K_{p, \beta, \lambda} = \alpha^2 K_{p, \alpha\beta, \alpha\beta}$  (see Equations 74 and 30). Then,  $\bar{\lambda} > 1$  and thus  $K_{p, \mathfrak{T}_p(\beta, \lambda)} = \bar{\alpha}^2 K_{p, \bar{\alpha}\bar{\beta}, 1 + \bar{\alpha}(\bar{\lambda} - 1)}$  (see Equations 77 and 30, where  $\alpha$  is here denoted by  $\bar{\alpha}$  and  $(\beta, \lambda)$  is obviously replaced by  $(\bar{\beta}, \bar{\lambda})$ ). Simple algebraic manipulations allow us to see that  $\bar{\alpha} = \frac{\lambda}{\beta}$  and that  $\mathfrak{T}_p(\alpha\beta, \alpha\beta) = (\bar{\alpha}\bar{\beta}, 1 + \bar{\alpha}(\bar{\lambda} - 1))$ , hence  $K_{p, \mathfrak{T}_p(\beta, \lambda)} = \left(\frac{\lambda}{\beta}\right)^2 K_{p, \mathfrak{T}_p(\alpha\beta, \alpha\beta)} = (\lambda\alpha)^2 K_{p, \alpha\beta, \alpha\beta}$  from Proposition 3. We then obtain again  $K_{p, \mathfrak{T}_p(\beta, \lambda)} = \lambda^2 K_{p, \beta, \lambda}$ . The case  $\lambda > 1$  is treated in a similar way, leading to the same conclusion.

### C.4 Explicit Expression of the Lower Bound.

Let us first consider the case  $\lambda < 1$ . Thus,  $\zeta_{p, \beta, \lambda} = \beta$  (see Equation 37). From Equations 74 and 75 and Equation 30, we have

$$\begin{aligned} K_{p, \beta, \lambda} &= \alpha^2 K_{p, \alpha\beta, \alpha\beta} \\ &= \frac{(\alpha\beta)^2 K_{p, \alpha\beta, \alpha\beta}}{\beta^2} \end{aligned}$$

that is, noting that  $\alpha\beta = \frac{\zeta_{p, \beta, \lambda}}{\zeta_{p, \beta, \lambda} + |1 - \lambda|}$ ,

$$K_{p, \beta, \lambda} = \frac{\left(\frac{\zeta_{p, \beta, \lambda}}{\zeta_{p, \beta, \lambda} + |1 - \lambda|}\right)^2 K_{p, \frac{\zeta_{p, \beta, \lambda}}{\zeta_{p, \beta, \lambda} + |1 - \lambda|}, \frac{\zeta_{p, \beta, \lambda}}{\zeta_{p, \beta, \lambda} + |1 - \lambda|}}}{\zeta_{p, \beta, \lambda}^2}, \tag{86}$$

when  $\lambda > 1$ . Thus,  $\zeta_{p, \beta, \lambda} = \beta + \frac{\lambda - 1}{p^*}$  (see Equation 37). Denoting  $(\bar{\beta}, \bar{\lambda}) = \mathfrak{T}_p(\beta, \lambda)$  (see Equation 11) and noting that  $\bar{\lambda} = \frac{1}{\lambda} < 1$  and applying successively Equation 13 (see previous subsection), Equations 74, 75 and 30

(where  $\alpha$  is denoted here  $\bar{\alpha}$  and  $(\beta, \lambda)$  is obviously replaced by  $(\bar{\beta}, \bar{\lambda})$ ), we have

$$\begin{aligned} K_{p,\beta,\lambda} &= \frac{1}{\lambda^2} K_{p,\bar{\beta},\bar{\lambda}} \\ &= \frac{(\bar{\alpha}\bar{\beta})^2 K_{p,\bar{\alpha}\bar{\beta},\bar{\alpha}\bar{\beta}}}{\lambda^2 \bar{\beta}^2}. \end{aligned}$$

It is straightforward to see that  $\lambda^2 \bar{\beta}^2 = \beta + \frac{\lambda-1}{p^*} = \zeta_{p,\beta,\lambda}$  and that  $\bar{\alpha}\bar{\beta} = \frac{p^*\beta+\lambda-1}{p^*\beta+\lambda-1+p^*(\lambda-1)} = \frac{\zeta_{p,\beta,\lambda}}{\zeta_{p,\beta,\lambda}+|\lambda-1|}$  so that Equation 86 still holds.

The case  $\lambda = 1$  can be viewed as the limit case, or using Equations 80 and 30 to conclude that Equation 86 still holds. It remains to evaluate  $l^2 K_{p,l,l} = l^2 C_{p,l,l}(g_{p,l})$  with  $l \leq 1$ . The evaluation of  $\sqrt{N_l(g_{p,l})}$  and  $\sqrt{F_{p,l}(g_{p,l})}$  was conducted for instance in [34], which gives with our notations, for  $l < 1$

$$l^2 K_{p,l,l} = \left[ \frac{2}{p^*} \left( \frac{p^*l}{1-l} \right)^{\frac{1}{p^*}} \left( \frac{p^*l}{(p^*+1)l-1} \right)^{\frac{l}{1-l} + \frac{1}{p}} B \left( \frac{1}{p^*}, \frac{1}{1-l} - \frac{1}{p^*} \right) \right]^2 \quad (87)$$

and

$$K_{p,1,1} = \left[ \frac{2 e^{\frac{1}{p^*}} \Gamma \left( \frac{1}{p^*} \right)}{p^* \frac{1}{p}} \right]^2. \quad (88)$$

Noting that  $\frac{1}{1-l} - \frac{1}{p^*} = \frac{l}{1-l} + \frac{1}{p}$  and taking  $l = \frac{\zeta_{p,\beta,\lambda}}{\zeta_{p,\beta,\lambda}+|1-\lambda|}$ , we achieve the wanted result from Equation 86.

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## Part III

# Conclusions and open problems

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Let us now give some conclusions and open problems associated with the contributions of this Thesis to the complexity and entropic uncertainty of the multidimensional Coulomb and harmonic systems of hydrogenic and oscillator types, and the generalized Planck distribution which governs the blackbody radiation in standard and non-standard universes.

First, we have obtained the Rényi and Shannon uncertainty measures for the ground and excited multidimensional hydrogenic states in terms of the dimensionality of the associated configuration space, the nuclear charge of the system and the hyperquantum numbers which characterize the states' wavefunctions. They have been expressed in a closed form by means of some multivariate hypergeometric functions of Lauricella and Srivastava-Daoust types. Special care has been taken for the high-energy (Rydberg) states and the high-dimensional (quasiclassical) states. The leading term of Rényi and Shannon entropies have been given for these two large groups of extreme states in a simple and compact way by using some recent ideas and techniques extracted from the modern approximation theory, which allow to determine the asymptotics of some power and logarithmic functionals (i.e., modified weighted  $\mathcal{L}_q$ -norms) of Laguerre and Gegenbauer polynomials when the polynomial degree or the parameter of their associated weight function becomes very large, respectively. It is worth mentioning that the optimal bound for the position-momentum Rényi-entropy-based uncertainty relations of Bilaynicki-Birula-Zozor-Vignat [91–93] is reached in the high-dimensional limit. For further details see Chapter 2 and the author's publications [31, 63, 70].

Second, we have analytically determined the Rényi and Shannon entropies for the multidimensional harmonic states in terms of the dimensionality of the associated configuration space, the oscillator strength and the hyperquantum numbers which characterize the states. The exact expressions for the Rényi and Tsallis entropies with integer parameter greater than unity have been found through the decomposition of the wave function in their Cartesian coordinates and by means of the Lauricella functions. On the other hand we have focused on the high-energy (Rydberg) states and the high-dimensional (pseudoclassical) states by use of the mathematical tools already described in the hydrogenic case. Remarkably, saturation of the position-momentum Rényi-entropy-based uncertainty relations of Bilaynicki-Birula-Zozor-Vignat [91–93] is reached in the high-dimensional limit, similarly to the hydrogenic case. For further details see Chapter 3 and the author's publications [64–66].

Third, the Crámer-Rao and Fisher-Shannon complexity measures have been respectively extended until a  $q$ -Gaussian context by using the generalized Crámer-Rao and Stam biparametric inequalities of Lutwak et al. [119]. The basic properties of these complexity quantifiers, including their behavior under replication transformation, have been discussed. The utility of these quantities have been shown for the  $d$ -dimensional blackbody frequency distribution at temperature  $T$ . We have found that they are universal constants in the sense that they are dimensionless and they do not depend on the

temperature nor on any physical constant (such as e.g., Planck constant, speed of light or Boltzmann constant), so that they only depend on the spatial dimensionality of the universe. For further details see Chapter 5 and the author's publications [67, 68].

Fourth, we have defined the notion of differential-escort transformation of a univariate probability density, and discussed its main properties. A linear law for the Shannon entropy of the differential-escort density, as well as a pseudo-linear law for the Rényi and Tsallis entropies through a rescaling of the entropic parameter have been found. We have determined the convexity behaviour of the Rényi entropy of a differential-escort density on the associated parameter, what in turn has allowed us to prove the monotonicity of the LMC-Rényi complexity measure with respect to the differential-escort transformations. Moreover, this control over the LMC-Rényi monotonicity has allowed us to study the entropic and complexity behaviour of a differential-escort density when it is strongly deformed to the low and high-complexity limits. Finally, we have applied the differential-escort transformation to the exponential and Tsallis  $q$ -exponential densities. We have found that the full family of  $q$ -exponential densities can be obtained as the differential escort transformations of the exponential density. Moreover, the application of this transformation to power-law decaying densities has allowed us (i) to show the capability of the differential-escort transformations to dramatically change the behaviour of the tail of the deformed distribution, and (ii) to propose a characterization for such densities. For further details see Chapter 6 and the author's publication [71].

Fifth, we have defined the triparametric Fisher-Rényi complexity measure for univariate probability densities and proven its basic properties. We have shown the regular behaviour of the one-dimensional biparametric Fisher information with respect to the differential-escort transformations. We have generalized the Stam inequality to a triparametric case for univariate probability densities by using two complementary methodologies: Gagliardo-Nirenberg inequalities and differential-escort densities. The latter one allows us to find an explicit expression for the optimal bound, as well as for the family of minimizing densities, namely the generalized  $(p, \beta, \lambda)$ -Gaussian densities. Moreover, the differential-escort methodology allows us to enlarge the validity domain beyond the one that Gagliardo-Nirenberg methodology can provide. We have numerically studied the triparametric Fisher-Rényi complexity measure for the radial density of the harmonic and hydrogenic systems at the lowest energy states. For further details see Chapter 7 and the author's publication [69].

Finally, let us enumerate a few open problems which we have identified during the realization of this dissertation:

- To find the exact expression of the Shannon entropy of the hydrogenic and harmonic systems for general stationary states. The techniques of Part I seem not to be powerful enough to determine it.

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- To determine the momentum Rényi entropy for the hydrogenic systems in the high-energy limit. We think that the use of the strong asymptotics of Aptekarev-Dehesa-Martinez-Finkelshtein [47] for the  $\mathcal{L}_p$ -norm of Gegenbauer polynomials might be useful to solve this open problem. In such a case, the Rényi-entropy-based uncertainty relation could be determined in the pseudo-classical limit.
  - To calculate rigorously the asymptotic behaviour of the Shannon entropy for both hydrogenic and harmonic systems in the pseudo-classical limit. Note that, although Rényi entropy is calculated for real values of the entropic parameter  $\lambda$ , the approximation method just fails when it is closed to unity, what prevents us from taking the limit  $\lambda \rightarrow 1$ .
  - To explore for both hydrogenic and harmonic systems the behaviour of the Rényi and Shannon entropies in the exceptional case when both dimensionality and principal hyperquantum number are simultaneously large.
  - To determine the Rényi entropy for the multidimensional harmonic systems in the hyperspherical formalism.
  - To extend the entropic study of the multidimensional harmonic system to oscillator-like systems with minimal length, which seem to play a relevant role for the consideration of quantum-gravity effects in uncertainty relations [271, 272].
  - To generalize the Fisher-information-based uncertainty relation by using the biparametric Fisher information here considered.
  - To solve the biparametric Fisher information for both hydrogenic and harmonic systems. This would allow us to obtain the exact expression of the generalized Crámer-Rao and Fisher-Rényi complexity measure, at least for a range of the entropic parameters.
  - To study the monotonicity property of the generalized complexity measures of Crámer-Rao and Fisher-Rényi types.
  - To extend the notion of differential-escort transformation for general multivariate distributions, but this seems to be a formidable task.
  - To generalize the triparametric Stam inequality to a general multivariate case. Neither the Gagliardo-Nirenberg inequality (since it does not give the optimal bound) nor the differential-escort methodology (see the previous open problem) are the appropriate ones for this extension.
  - To extend the biparametric Crámer-Rao inequality to a triparametric case by means of a Stam-like procedure.

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